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Diffractive optics with harmonic radiation in 2d nonlinear photonic crystal waveguide

Vincent Lescarret and Guido Schneider

Abstract. The propagation of modulated light in a 2d nonlinear photonic waveguide is investigated in the framework of diffractive optics. It is shown that the dynamics obeys a nonlinear Schrödinger equation at leading order. We compute the first and second corrector and show that the latter may describe some dispersive radiation through the structure. We prove the validity of the approximation in the interval of existence of the leading term.

Contents

1. Introduction

Periodic media such as metallic crystals and semi-conductors have drawn scientists' attention because of their band-gap spectrum which accounts for their strong dispersive properties. In the range of optical wavelengths we find the Photonic Crystals (PhC) whose popularity is partly due to the small sizes and the possibility to slow down the light. We refer the reader to the quite exhaustive report [6] on PhC. Because the spectrum gives a good hint on the way waves propagate, the research on these materials mostly focuses on this aspect (see [13, 14, 15, 17, 18]). However, as pointed out in [31] the spectrum alone does not explain the wave resonance and wave radiation in a medium. Such effects are not harmonic in time and are indeed observed in nonlinear media when one lets a wave evolve from an initial state close but not equal to an eigenvalue.

With this idea in mind we address the issue of computing and analyzing the propagation of an electromagnetic pulse in 2d, straight, nonlinear PhC waveguides (see Figure 1.1). The guides are made of a PhC from which a finite number of rows is removed. The spatial extent of the pulse envelope may be of the order of a few cells of periodicity of the PhC or much larger along the direction of the guide. We denote by η the periodicity of the cell divided by the spatial length of the pulse envelope. The nonlinear response of the PhC makes possible the existence of solitons whose shape and energy are preserved and is responsible for harmonics (third harmonics in centro-symmetric media) which may radiate part of the energy. We consider this issue in the framework of diffractive optics (see [11]), that is, for times of order $1/\eta^2$ for which one can observe the soliton propagating and the third harmonic radiating. The main goal of this study is to mathematically describe this harmonic radiation and the way it disturbs the soliton.

This situation is quite academic but brings new results in (mathematical) nonlinear optics for PhC. The case of linear optics in homogeneous PhC was addressed in [9]. Then, in the framework of nonlinear diffractive optics, the author in [8] derived a Nonlinear Schrödinger equation (NLS) as a model for propagation of waves in 1d PhC. This was extended by [4] in a multi-dimensional setting but still for homogeneous PhC.

The present analysis relies on the spectral properties of the waveguide which are precisely given in the next sections. In particular we provide a resolution of identity of a class of transverse operators modeling the situation. It is mainly based on A. Figotin, P. Kuchment and coauthors' work, and more precisely on [16]. It can be seen as a continuation of [3] as well. We use a WKB (also called WKBJ) asymptotic expansion to compute the leading part of the field and the two first correctors involving the third harmonic. There are two difficulties. The first one is due to the discontinuous nature of the PhC. We thus deal with quasilinear PDEs with discontinuous coefficients, whose analysis leads us to restrict our considerations to PhC periodic in one direction and homogeneous in the other one. We comment on this lack of generality in the conclusion, giving some insights in the problems which one faces otherwise. The second difficulty comes from the third harmonic when it is a point of the essential spectrum of the underlying operator. The amplitude is a solution of a Helmholtz-like singular equation, whose resolution needs a new Ansatz, which transforms the equation into a non-autonomous wave equation with source term. According to [28] the solution may grow secularly in time. We thus analyze the equation in detail and show that the energy is bounded by $\log(\eta)$ for diffractive times, which validates the WKB analysis in the diffractive regime.

1.1. Modelisation and assumptions

The propagation of light in a photonic waveguide is described by Maxwell's equations in dielectric but non-magnetic medium:

$$\mathbf{rot}\,\mathbf{H} - \partial_t \mathbf{D} = 0, \qquad \mathbf{rot}\,\mathbf{E} + \partial_t \mathbf{B} = 0, \tag{1.1}$$

$$\nabla \cdot \mathbf{D} = 0, \qquad \nabla \cdot \mathbf{B} = 0, \tag{1.2}$$

$$\mathbf{D} = \varepsilon(\mathbf{E} + \mathbf{P}), \qquad \mathbf{B} = \mu_0 \mathbf{H} \tag{1.3}$$

where ε is the dielectric permittivity of the medium and μ_0 the magnetic permeability of vacuum.

Assumption 1.1. *The dielectric permittivity ε is assumed to be positive.*

A bi-dimensional photonic waveguide can be seen as a 2d periodic medium possessing a row of defects spreading in the x direction (see Figure 1.1). The permittivity thus reads as $\varepsilon = \varepsilon_0(x, y) + \tilde{\varepsilon}(x, y)$ where ε_0 is periodic and $\tilde{\varepsilon}$ is compactly supported with respect to y. Moreover ε is piecewise continuous, typically piecewise constant.

For small electric fields and centro-symmetric media the polarization $\mathbf{P}$ can be expanded into an odd power series of the electric field. Here, for simplicity we take

$$\mathbf{P} = \chi_3 |\mathbf{E}|^2 \mathbf{E}. \tag{1.4}$$

Because of the technical difficulties related to general potentials of two variables we will assume further

Assumption 1.2. *ε_0 and $\tilde{\varepsilon}$ only depend on y and $supp\,\tilde{\varepsilon} = [-a, a]$. Similarly χ_3 only depend on y. Finally we assume that $\tilde{\varepsilon}$ keeps the same sign in $[-a, a]$.*

This assumption is used at two stages in this paper: for the description of the transverse operator (see Lemma 2.5) and for the nonlinear analysis which is needed to study the convergence of the approximate solution which we next compute, towards a (related) exact one (see Section 2.3). See Section 3 for some comments.

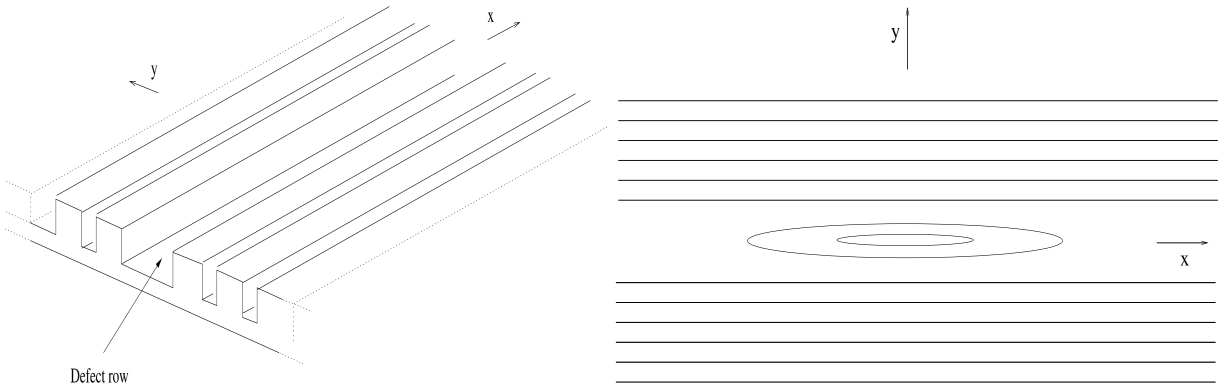

FIGURE 1. PhC waveguide satisfying Assumption 1.2.

In 2d one can distinguish two sub-cases: $\mathbf{E} = (E_1, E_2, 0)$ and $\mathbf{E} = (0, 0, E_3)$. In the first case we have with $U = {}^t(E_1, E_2, B_3)$

$$\partial_t U + \begin{pmatrix} 0 & 0 & -1/\varepsilon\partial_y \\ 0 & 0 & 1/\varepsilon\partial_x \\ \partial_x & -\partial_y & 0 \end{pmatrix} U = \chi_3 \partial_t \begin{pmatrix} |\mathbf{E}|^2 E_1 \\ |\mathbf{E}|^2 E_2 \\ 0 \end{pmatrix}$$

In the second case, setting $U = {}^t(E_3, B_1, B_2)$ we get

$$\partial_t U + \begin{pmatrix} 0 & -1/\varepsilon\partial_x & 1/\varepsilon\partial_y \\ \partial_y & 0 & 0 \\ -\partial_x & 0 & 0 \end{pmatrix} U = \chi_3 \partial_t \begin{pmatrix} E_3^3 \\ 0 \\ 0 \end{pmatrix}$$

Remark that the last system is nonlinear only with respect to E_3:

$$\partial_t^2(E_3 + \chi_3 E_3^3) - \frac{1}{\varepsilon}\Delta E_3 = 0, \qquad \Delta = \partial_x^2 + \partial_y^2. \tag{1.5}$$

Thus no divergence condition is needed. The magnetic field is then given by $\partial_t \mathbf{B} + \mathrm{rot}\mathbf{E} = 0$. Equation (1.5) is a nonlinear version of the so-called transverse electric (TE) equation. Because of its simplicity we focus our analysis on equation (1.5) and give some comments for the transverse magnetic (TM) case in section 3. However, it should be noticed that the equation for U is conservative but equation (1.5) is not.

In the next section we investigate precisely how electromagnetic pulses propagate, disperse and undergo the nonlinear effects along the guide. We carry out the subsequent analysis within the framework of the diffractive optics, using WKB expansions.

For the reader convenience we present all our results in the next section with rather short proofs or hint of proofs and postpone the longer ones in Appendix.

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2. Diffractive optics of TE modes in 2d nonlinear Photonic crystal waveguide

We intend to investigate the regime of weakly nonlinear diffractive optics for a wave propagating along the defect. We thus give ourself an initial data for (1.5) of the form

$$E(t=0) = \eta A(\eta x, y) e^{ikx},$$

where E is in fact E_3, η is the small parameter defined in the introduction and A is the envelope (also called profile) which does not depend on η. Note that the crystal periodicity and the wavelength are of comparable order. The variable ηx accounts for the shape of the envelope. In the following we will determine k so that the solution of (1.5) with the above initial data is in $L^2(\mathbb{R}^2)$. This will be performed by looking first for the eigenmodes of the linear operator involved in equation (1.5) which are localized around the defect. Such modes exist under a geometric assumption similar to the one given by [13]. Those results are given in Lemma 2.5.

We look for an exact solution of (1.5) as a WKB expansion :

$$E(t,x,y) = \eta E^\eta(\underbrace{\eta^2 t}_{T}, \underbrace{\eta(x-vt)}_{X}, x, y, t), \quad E^\eta = \sum_{j\geq 0} \eta^j E_j \,. \tag{2.1}$$

The profiles E_j are function of T, X, x, y, t. It is well known (see [11]) that the envelope of the wave propagates and X keeps track of it. The the group velocity v is to be determined so that E solves accurately (1.5). This was already done in [9] and does not involve the nonlinear part of the polarization. The variable T allows to describe the evolution of the envelope for distances much greater than the size of the envelope.

Replacing E by its expression in term of E^η in (1.5) leads

$$\begin{aligned}(\partial_t^2 - \frac{1}{\varepsilon}\Delta)E^\eta - 2\eta(v\partial_t + \frac{1}{\varepsilon}\partial_x)\partial_X E^\eta + 2\eta^2(\partial_T\partial_t + (v^2 - \frac{1}{\varepsilon})\partial_X^2)E^\eta - 2v\eta^3\partial_X\partial_T E^\eta + \eta^4\partial_T^2 E^\eta = \\ - \eta^2\chi_3\Big(\partial_t^2 - 2v\eta\partial_X\partial_t + \eta^2(v^2\partial_X^2 + 2\partial_T\partial_t) - 2v\eta^3\partial_X\partial_T + \eta^4\partial_T^2\Big)(E^\eta)^3. \quad (2.2)\end{aligned}$$

Next, replacing E^η by the series and canceling the coefficients in front of η^j, $j \leq 2$ yields a set of equations whose first three are:

$$\begin{aligned}&(\partial_t^2 - \frac{1}{\varepsilon}\Delta)E_0 = 0, \\ &(\partial_t^2 - \frac{1}{\varepsilon}\Delta)E_1 - 2(v\partial_t + \frac{1}{\varepsilon}\partial_x)\partial_X E_0 = 0, \\ &(\partial_t^2 - \frac{1}{\varepsilon}\Delta)E_2 - 2(v\partial_t + \frac{1}{\varepsilon}\partial_x)\partial_X E_1 + 2(\partial_T\partial_t + (v^2 - \frac{1}{\varepsilon})\partial_X^2)E_0 = -\chi_3\partial_t^2(E_0^3)\,.\end{aligned} \tag{2.3}$$

The strategy is to solve each equation in the given order to get an approximation of the exact solution of (1.5). We look for harmonic profiles in t, x with pulsation ω and wave number k. The first equation thus requires to compute the kernel of the operator $M(k) - \omega^2$ with

$$M(k) := -\frac{1}{\varepsilon}(\partial_y^2 - k^2), \tag{2.4}$$

defined through its quadratic form in a H^1-weighted space for which the operator is self-adjoint, see Notation 2.3. The existence of a guided mode is equivalent to the existence of a non-zero kernel which one can ensure for some k, ω under geometrical conditions (see Lemma 2.5). The amplitude of the leading term thus belongs to $\ker(M(k) - \omega^2)$; we say it is polarized. Denoting by $\Pi(k)$ the orthogonal projector on $\ker(M(k) - \omega^2)$ (see Definition 2.7), the second equation leads the speed v together with the constraint

$$\Pi(k)(v\omega + \frac{k}{\varepsilon})\Pi(k) = 0.$$

Thanks to this relation the leading term and the first corrector decouple. Then, the third equation shows that the leading profile is solution of a nonlinear Schrödinger equation whose coefficients are some homogenized quantity involving ε.

Next, to achieve the convergence of E_0 towards the exact solution of Equation (1.5), one needs to compute the corrector up to E_2. But because of the nonlinear terms, solving the third equation requires to distinguish two cases:

- $9\omega^2 \in \mathrm{Res}(M(3k))$ (resolvent set of $M(3k)$), then the third harmonic of E_2 is purely oscillating,
- $9\omega^2 \notin \mathrm{Res}(M(3k))$, then the third harmonic of E_2 radiates (through a dispersion process).

Before stating the main result we need to introduce the space in which we analyze equation (1.5). Using Assumption 1.2 we define inhomogeneous spaces like [19] with limited regularity in y but unlimited in x:

Definition 2.1. *For $s \in \mathbb{N}$ and $T \geq 0$ define*

$$\mathcal{H}^s(T) := \bigcap_{j=0}^{s} \mathcal{C}^j([0,T]; H^{s-j,1}(\mathbb{R}^2)), \quad \textit{with} \quad H^{k,1}(\mathbb{R}^2) = \{u \mid \partial_y^a \partial_x^b u \in L^2(\mathbb{R}^2),\ a \leq 1,\ a+b \leq k\}.$$

For $T < 0$ replace $[0,T]$ by $[T,0]$.

For any set Ω we also denote by $H^s(\Omega)$ the usual Sobolev space of functions which have s-derivative in $L^2(\Omega)$. In Lemma 2.18 we show that $\mathcal{H}^2(T)$ is an algebra. This property is needed for the convergence analysis using the quasilinear equation (1.5). The main result can be formulated as follows:

Theorem 2.2. *Assume the operator given by* (2.4) *possesses an eigenvalue ω^2 for some $k \neq 0$. One can construct a WKB approximate solution of Equation* (1.5)*:*

$$E_{app} = \eta(E_0 + \eta E_1 + \eta^2 E_2)$$

with $E_0(t,x,y) = \mathcal{A}_0(\eta^2 t, \eta(x - vt))w_0(y)e^{i(\omega t + kx)}$ where w_0 is the eigenfunction of (2.4) *associated to ω^2 and $\mathcal{A}_0$ is solution of a nonlinear Schrödinger equation (see Eq.* (2.9)*). So, there is a $T_0 > 0$ such that if $\mathcal{A}_0(T=0) \in H^{2s}(\mathbb{R})$ then $\mathcal{A}_0 \in \cap_j \mathcal{C}^j(0,T; H^{2s-j}(\mathbb{R}))$.*

Then, $(1 - \Pi(k))E_1$ is determined from E_0. Next, for E_2 there are two possibilities: if $9\omega^2 \in Res(M(3k))$, then

$$E_2 = A_{2,1}(T,X,y)e^{i(\omega t + kx)} + A_{2,3}(T,X,y)e^{3(i\omega t + kx)} + c.c.$$

(see Formulas in Subsection 2.2.1 *for the expression of the coefficients $A_{2,1}, A_{2,3}$), while if $9\omega^2 \notin Res(M(3k))$ then*

$$E_2 = A_{2,1}(T,X,y)e^{i(\omega t + kx)} + A_{2,3}(T,X,t,y)e^{3(i\omega t + kx)} + c.c.,$$

where $A_{2,3}$ is solution of a non autonomous wave equation in the variables t, y (see Equation (2.12)*). Finally, for $s \geq 3$ there exists $\eta_0 > 0$ such that for any $\eta \leq \eta_0$ Equation* (1.5) *with initial data*

$$E(t=0) = E_{app}(t=0) + \eta^{3/2} G_1, \quad \partial_t E(t=0) = \partial_t E_{app}(t=0) + \eta^{3/2} G_2,$$

where $G_1 \in H^{2,1}$ and $G_2 \in H^{1,1}$ possesses a solution

$$E = E_{app} + f(\eta)\eta^{3/2} R,$$

where $f(\eta) = 1$ if $9\omega^2 \in Res(M(3k))$ and $f(\eta) = -\ln(\eta)$ otherwise and the remainder R belongs to $\mathcal{H}^2(T_0/\eta^2)$.

Let us point out that we do not solve the initial value problem for (1.5) in general but for specific solutions with well-tuned initial values. However, those solutions are among the most interesting ones since they describe the propagation of a guided wave (solitons). Most other initial values give rise to solutions which do not propagate but disperse in the guide.

2.1. Spectral analysis

First consider the leading term under the form

$$E_0 = A_0(y)\mathcal{E} + c.c., \quad \mathcal{E} = e^{i(\omega t + kx)}. \tag{2.5}$$

We do not consider the slow variables since they appear as parameters in the first equation. With this Ansatz and using the notation (2.4), the first equation of the cascade (2.3) becomes

$$(\omega^2 - M(k))A_0 = 0. \tag{2.6}$$

Notations 2.3. *Define* $L^2_\varepsilon(\mathbb{R})$ *through the scalar product* $(u,v)_\varepsilon = \int_{\mathbb{R}} \varepsilon u\bar{v}dy$. *Also denote by* $\|\cdot\|_\varepsilon$ *the related norm. Let us denote by* $H^1_\varepsilon(\mathbb{R})$ *the usual Sobolev space endowed with the scalar product* $(u,v)_\varepsilon + (\nabla u, \nabla v)_\varepsilon$. *We use the notation* $\|\cdot\|_2$ *and* $(,)$ *when the weight is* 1.

The properties of the fiber operator $M(k)$ are summarized in the next lemma which follows from [13, 14, 15, 17, 18]. Let us denote by $M_0(k)$ the unperturbed operator, i.e. when $\tilde{\varepsilon} = 0$. For this operator the Floquet-Bloch theorem is a fundamental tool:

Definition 2.4. *For* $x \in \mathbb{R}^n$ *define the Floquet-Bloch transform of a function* $f \in L^2_{\varepsilon_0}(\mathbb{R}^n)$ *by*

$$\widetilde{f}(x,\ell) = \sum_{j\in\mathbb{Z}^n} \hat{f}(\ell + j)e^{ijx}, \quad \ell \in [-1/2, 1/2)^n.$$

Here $\hat{f}$ *is the Fourier transform of* f *in* $\mathbb{R}^n$. *The Floquet-Bloch transform possesses an inverse given by*

$$f(x) = \int_{[-1/2,1/2]^n} e^{i\ell x}\widetilde{f}(x,\ell)d\ell \ .$$

Moreover one has the Parseval-like identity $\|f\|_{L^2_{\varepsilon_0}(\mathbb{R}^n)} = \|\widetilde{f}\|_{L^2_{\varepsilon_0}([0,2\pi]^n\times[-1/2,1/2]^n)}$.

In the next Lemma we use Reed-Simon's decomposition of the spectrum $\sigma(A)$ of an operator A: $\sigma(A) = \sigma_p(A) \cup \sigma_{ess}(A)$ where $\sigma_p(A)$ is the set of isolated and finite geometric multiplicity eigenvalues of A and $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_p(A)$. In turn, the essential spectrum is split in three disjoint sets: the absolutely continuous spectrum, the set of eigenvalues with infinite multiplicity and the residual spectrum.

Lemma 2.5. *Under Assumption* 1.2 *there holds*

1. $M_0(k)$ *is self-adjoint in* $L^2_{\varepsilon_0}(\mathbb{R})$ *and has a band-gap spectrum, i.e. its spectrum is reduced to the absolutely continuous spectrum and is a union of intervals.*
2. $\sigma_{ess}M(k) = \sigma_{ess}M_0(k)$.
3. *The eigenvalues of* $M(k)$ *are situated in the gaps of* $M_0(k)$ *and there is a finite number of them in each gap.*
4. *If the spectrum of* $M_0(k)$ *possesses a gap* (λ_a, λ_b) *then, choosing* $(a \inf_{]-a,a[}\tilde{\varepsilon})$ *large enough,* $M(k)$ *possesses at least an eigenvalue* $\lambda_0 \in (\lambda_a, \lambda_b)$.
5. *A corresponding eigenfunction* w_0 *belongs to* $H^1_\varepsilon(\mathbb{R}) \cap H^2(\mathbb{R})$. *Moreover it decays exponentially.*

We give a hint of proof for the first point of the lemma and by the way we introduce the "band functions" which allow to describe the spectrum of $M_0(k)$. This property is proved in [12], Theorem 5.3.2 or [30], Theorem XIII.86.

It is clear that $M_0(k)$ is self adjoint in $L^2_{\varepsilon_0}(\mathbb{R})$. The fact that it possesses a band-gap spectrum is shown by using the Floquet-Bloch transform. Indeed

$$M_0(k)f(y) = \int_{-1/2}^{1/2} e^{iy\ell}M_0(k,\ell)\widetilde{f}(y,\ell)d\ell,$$

where $M_0(k,\ell)$ is the operator $M_0(k)$ replacing ∂_y by $\partial_y + i\ell$ and defined in the space of square integrable and y-periodic functions (since $\widetilde{f}$ has both properties). Thus $M_0(k,\ell)$ has a compact resolvent and we denote by $e_j(k,\ell), \lambda_j(k,\ell)$ its eigenvectors and eigenvalues. One thus gets a spectral representation for $M_0(k,\ell)$ and therefore for $M_0(k)$ too, so one sees that $\sigma(M_0(k))$ is absolutely continuous and

$$\sigma(M_0(k)) = \bigcup_{j>0}\{\lambda_j(k,\ell), \quad \ell \in [-1/2,1/2]\}. \tag{2.7}$$

We postpone the remaining proof of the lemma to Appendix A.

We point out that we do not know in general how many eigenvalues $M(k)$ has and in which gaps. However, for small perturbations, it is possible to compute the way the eigenvalues evolve in term of the strength κ of the perturbation and estimate their number ([5, 10]). One can also compute an expansion (in term of κ) of the closest eigenvalue to an end of a gap ([7]).

When the fourth point of the lemma is fulfilled the PhC waveguide possesses a guided mode. If not, there is no hope that the light be guided along the defect. We thus assume that such a guided mode exists.

Assumption 2.6. *There exists a k such that $M(k)$ possesses at least an eigenvalue ω_0^2 situated in a gap (λ_a, λ_b). We also assume that ω_0^2 is simple.*

Let us call $w_0(k, y)$ the associate eigenvector. It is real, for it solves the real coefficient equation (2.6). Thanks to the third point of the previous lemma ω_0^2 is separated from the remaining part of the spectrum of $M(k)$. This allows to define a projector and a partial inverse as follows:

Definition 2.7. *Let $\Pi(k)$ be the orthonormal projector on $ker(M(k) - \omega_0^2)$. Thus $\Pi(k)u = (w_0, u)_\varepsilon w_0$. Then let $Q(k)$ be the symmetric partial inverse of $M(k) - \omega_0^2$ vanishing on $ker(M(k) - \omega_0^2)$.*

Those objects are used to analyze the three equations for the profiles.

2.2. Solving the equation for the profiles

The first equation in (2.3) is already solved in the previous paragraph: E_0 is given by (2.5) but it is now considered as a function depending on T, X and y and we set $A_0(T, X, y) = \mathcal{A}_0(T, X)w_0(y)$ where $\mathcal{A}_0$ will be determined by the next equations. Note that $A_0 = \Pi(k)A_0$.
Turning to the second equation, we look for E_1 like E_0 under the form $A_1(T, X, y)\mathcal{E} + c.c.$ where we recall that $\mathcal{E} = e^{i(\omega t+kx)}$ and A_1 is decaying exponentially with respect to y. The second equation in (2.3) thus reads

$$(-\omega_0^2 + M(k))A_1 + i(\omega_0 v + \frac{k}{\varepsilon})\partial_X A_0 = 0 \ .$$

Applying $\Pi(k)$ yields $\Pi(k)(\omega_0 v + \frac{k}{\varepsilon})\partial_X A_0 = 0$ from which we get

$$v = -\frac{k}{\omega_0}\|w_0\|_2^2/\|w_0\|_\varepsilon^2, \quad \text{and} \quad \Pi(k)(\omega_0 v + \frac{k}{\varepsilon})\Pi(k) = 0.$$

Thus

$$A_1 = \Pi(k)A_1 - iQ(k)(\omega_0 v + \frac{k}{\varepsilon})\partial_X A_0.$$

The unknown term $\Pi(k)A_1$ is given similarly as A_0 by $\mathcal{A}_1 w_0$ where $\mathcal{A}_1$ is a function of T and X. Let us now consider the third equation. Here the nonlinearity shows up. We set

$$P_0 = \chi_3\omega_0^2 E_0^3 = P_{0,1}\mathcal{E} + P_{0,3}\mathcal{E}^3 + c.c..$$

Looking for

$$E_2 = A_{2,1}(T, X, y)\mathcal{E} + A_{2,3}(T, X, y)\mathcal{E}^3 + c.c.,$$

with A_2 decreasing exponentially w.r.t. y yields

$$(-9\omega_0^2 + M(3k))A_{2,3} = P_{0,3}.$$

Solving this equation depends whether $9\omega_0^2$ is a point of the discrete or essential spectrum of $M(3k)$ or a point of the resolvent set of $M(3k)$.

2.2.1. Non resonant third harmonic. Let us first assume

Assumption 2.8. $9\omega_0^2$ *belongs to the resolvent set of $M(3k)$.*

The assumption means that $9\omega_0^2 - M(3k)$ is invertible and thus

$$A_{2,3} = (-9\omega_0^2 + M(3k))^{-1}P_{0,3}.$$

Next, the first harmonic solves

$$(M(k) - \omega_0^2)A_{2,1} = P_{0,1} + \ 2i\left(\omega_0 v + \frac{k}{\varepsilon}\right)\partial_X A_1 - \ 2i\omega_0\partial_T A_0 \ - 2(v^2 - \frac{1}{\varepsilon})\partial_X^2 A_0. \qquad (2.8)$$

The left hand side is orthogonal to $\ker(M(k)-\omega_0^2)$. A resolubility condition is thus that the image by $\Pi(k)$ of the right hand side must vanish. Using the identity $\Pi(k)(\omega_0 v + k/\varepsilon)\Pi(k) = 0$ one gets

$$i\omega_0\partial_T\mathcal{A}_0 + R\partial_X^2\mathcal{A}_0 = \frac{1}{2}(P_{0,1}, w_0)_\varepsilon = \frac{\omega_0^2}{2}\mathcal{A}_0^3(\chi_3 w_0^3, w_0)_\varepsilon, \tag{2.9}$$

where

$$R = \left((v^2 - \frac{1}{\varepsilon})w_0, w_0\right)_\varepsilon - \left(Q(k)(\omega_0 v + \frac{k}{\varepsilon})w_0, (\omega_0 v + \frac{k}{\varepsilon})w_0\right)_\varepsilon \in \mathbb{R}.$$

Thanks to this resolubility condition, both sides of equation (2.8) belong to the orthogonal set of $\ker(M(k)-\omega_0^2)$. This allows to apply the partial inverse $Q(k)$:

$$(1-\Pi(k))A_{2,1} = Q(k)\left(P_{0,1} + \ i\left(\omega_0 v + \frac{k}{\varepsilon}\right)\partial_X A_1 - \ 2i\omega_0\partial_T A_0 \ - 2(v^2 - \frac{1}{\varepsilon})\partial_X^2 A_0\right). \tag{2.10}$$

Note that the last expression involves $\Pi(k)A_1 = \mathcal{A}_1 w_0$ where $\mathcal{A}_1$ is unknown. It would be determined by the next (fourth) equation in the cascade since it would lead a Schrödinger equation as for $\mathcal{A}_0$. But we do not need to do it since the order of approximation is sufficient (see Lemma 2.21) so we may take $\mathcal{A}_1(T,X)$ equal to its initial value, i.e. $\mathcal{A}_1(0,X)$. The same holds for $\Pi(k)A_{2,1}$ but since it is a second corrector we may take it equal to zero.

2.2.2. Weakly resonant third harmonic. Let us now assume $9\omega_0^2$ is weakly resonant in the following sense:

Assumption 2.9. *$9\omega_0^2$ belongs to the essential spectrum of $M(3k)$. From Lemma 2.5, $9\omega_0^2$ is not an eigenvalue of $M(3k)$.*

Remark 2.10. *Note that Assumption 2.9 is more likely to be fulfilled than Assumption 2.6 but it depends on the regularity of ε_0:*

- *If ε_0 is continuous, the gaps shrink thus Assumption 2.9 will be generically satisfied.*
- *if ε_0 is piecewise constant the gaps and the bands are of comparable measure thus both Assumption 2.6 and Assumption 2.9 are likely to be fulfilled. This can be seen in [21] where the spectrum for a particular Hill equation is computed (also see [12]).*

If we would remove Assumption 1.2 then one could still define an operator $M_0(k)$ (k would be a Bloch mode) and in this case Assumption 2.9 would be generically satisfied since there are fewer and smaller gaps in 2d periodic media than in 1d (see [25]).

This is typically the situation considered by Soffer and Weinstein [31]. They show that one cannot expect the harmonics to be purely time oscillating functions. Usually, one expects a complex resonant and dispersive process between the fundamental mode and the third harmonics. However, in our case, since the third harmonic shows up as a corrector (with respect to the small parameter η) its dispersion does not affect the leading term. The suitable Ansatz describing the situation is to let $A_{2,3}$ depend on t:

$$E_2 = A_{2,1}(T,X,y)\mathcal{E} + A_{2,3}(T,X,t,y)\mathcal{E}^3 + c.c.$$

This Ansatz does not modify the two first equations but only the third one which becomes:

$$\begin{aligned}(M(k)-\omega_0^2)A_{2,1}\mathcal{E} \ + \ \left((\partial_t + 3i\omega_0)^2 + M(3k)\right)A_{2,3}\mathcal{E}^3 - \ i\left(\omega_0 v + \frac{k}{\varepsilon}\right)\partial_X A_1\mathcal{E} \\ + \ i\omega_0\partial_T A_0\mathcal{E} \ + (v^2 - \frac{1}{\varepsilon})\partial_X^2 A_0\mathcal{E} + \ c.c. = P_{0,1}\mathcal{E} + P_{0,3}\mathcal{E}^3 + c.c..\end{aligned}$$

Projecting the equation on the basis $\exp(\pm ikx)$ and $\exp(\pm 3ikx)$ we get

$$(M(k)-\omega_0^2)A_{2,1} - \ i\left(\omega_0 v + \frac{k}{\varepsilon}\right)\partial_X A_1 + \ i\omega_0\partial_T A_0 \ + (v^2 - \frac{1}{\varepsilon})\partial_X^2 A_0 = P_{0,1}, \tag{2.11}$$

$$\left((\partial_t + 3i\omega_0)^2 + M(3k)\right)A_{2,3} = P_{0,3}. \tag{2.12}$$

The equation (2.11) is the same as (2.8). We thus get the same NLS equation for the leading profile. Let us now turn to Equation (2.12). It is a non-autonomous wave equation with time constant source term (T and X are considered as parameters). In order to be a valid corrector, the L^2 norm of $A_{2,3}$ has to be small compared to that of A_1/η for times of order η^{-2}. This property is satisfied if

$$\lim_{t\to\infty} \frac{1}{\sqrt{t}}\|A_{2,3}\|_2 = 0.$$

This behavior is reminiscent of the so-called under-linear growth criterion used in diffractive optics (see [27]). Unfortunately

Remark 2.11. *Taking the scalar product of* (2.12) *by* $\partial_t A_{2,3}$ *in* $L^2_\varepsilon(\mathbb{R})$*, using the Cauchy Schwarz inequality for the right hand side and integrating in time, we get*

$$\mathcal{N}(t) \le \mathcal{N}(0) + t\|P_{0,3}\|_\varepsilon,$$

$$\textit{with} \quad \mathcal{N}^2(t) = \|(\partial_t + 3i\omega_0)A_{2,3}\|^2_\varepsilon + \|\partial_y A_{2,3}\|^2 + 9k^2\|A_{2,3}\|^2.$$

The norm $\|\cdot\|$ *is the usual* $L^2(\mathbb{R})$ *norm.*

This simple argument shows that one cannot expect a bound independent of η for $t \sim T/\eta^2$ just by using $\|P_{0,3}\|_\varepsilon$. A refined analysis can be found in [28] in the case of autonomous hyperbolic systems. Actually such a tool does not apply directly but the concept of small resonance set does. The analysis of a similar equation has been done by [31] using the spatial decrease of the source term by the mean of Mourre-like estimates. Unfortunately such estimate require smooth coefficients (see the use of commutators in [29]). Instead, we use the spectral resolution of $M(k)$ and estimate directly the solution which we express with the Duhamel formula. By doing the analysis we need to precise the behavior of the $\lambda_j,\ j > 0$.

Lemma 2.12. *The functions* λ_j *are even on* $[-1/2, 1/2]$ *and strictly monotone and analytic on* $]0, 1/2[$*. Moreover they are simple except at the points* 0 *and* 1/2 *where they are at most double.*

Proof. The first part of the lemma is very similar to [30], Lemma XIII.89. We give the main idea: the evenness is because ε is real. Then for the other claims one needs to consider the discriminant $D(\omega)$ (see [12]) of the operator $M_0(k)$ which allows to compute the Floquet multipliers $\rho = e^{2i\pi\ell}$ and thus the Floquet exponent ℓ in term of ω according to the following equation $\rho^2 - D(\omega)\rho + 1 = 0$. From the expression of ρ one sees that it is complex if $D(\omega) \in [-2, 2]$ and real otherwise. In the first case the Floquet exponent is real and it describes a band of the spectrum while it is imaginary in the second case and describes a gap (resolvent set). Theorem (2.3.1) in [12] tells that $D(\omega)$ is a strictly monotone function when $|D(\omega)| < 2$. This implies the strict monotonicity of $\ell(\omega)$ on the range of λ_j (which describes a band) hence that of $\lambda_j(\ell)$. Moreover, if λ_j is increasing then $\lambda_{j\pm1}$ are decreasing. One concludes that λ_j is simple except at 0 and 1/2 where it might be double.

Next, the smoothness of λ_j on $]0, 1/2[$ is a direct consequence of the expression of ρ in term of $D(\omega)$ which is holomorphic. $\square$

We now formulate our last assumption whose aim is to compel the energy carried by the third harmonic to disperse. From Assumption 2.9 there are $j_0 > 0$ and ℓ_0 such that $9\omega_0^2 = \lambda_{j_0}(3k, \ell_0)$.

Assumption 2.13. *We assume that* ℓ_0 *is different from* 0 *and* $\pm 1/2$.

From the previous lemma we see that the assumption implies $\partial_\ell \lambda_{j_0}(3k, \ell_0) \neq 0$. If no λ_j are double at 0 nor 1/2 this assumption means that $9\omega_0^2$ is not a point of the boundary of $\sigma_{\mathrm{ess}} M(3k)$.

Lemma 2.14. *Under the Assumptions* 2.9 *and* 2.13*, the solution of Equation* (2.12) *with initial data in* $H^\infty_\varepsilon(\mathbb{R})$ *is such that for all* $a \in \mathbb{N}$ *there is a positive constant* $c(a, k)$ *independent of* t *such that*

$$\|\partial_t^a A_{2,3}(t)\|_\varepsilon + \|\partial_t^a \partial_y A_{2,3}(t)\|_\varepsilon \le c(a,k)\left(\|\partial_y^{a+1} A_{2,3}(0)\|_\varepsilon + \|\partial_y^a \partial_t A_{2,3}(0)\|_\varepsilon + (1 + \ln(t))\|(1 + |y|)^2 P_{0,3}\|_\varepsilon\right).$$

Idea of the proof. Since $M(3k)$ is self-adjoint in $L^2_\varepsilon(\mathbb{R})$ and positive, $\sqrt{-M(3k)} = \pm i\sqrt{M(3k)}$ is skew-adjoint. The related semi-group is well-defined and $A_{2,3}$ is given by the Duhamel formula:

$$A_{2,3} = e^{-3i\omega_0 t}\cos\left(t\sqrt{M(3k)}\right)A_{2,3}(t=0) + \frac{e^{-3i\omega_0 t}}{\sqrt{M(3k)}}\sin\left(t\sqrt{M(3k)}\right)\partial_t A_{2,3}(t=0)$$
$$+\frac{1}{\sqrt{M(3k)}}\int_0^t e^{3i\omega_0(s-t)}\sin\left((t-s)\sqrt{M(3k)}\right)P_{0,3}. \quad (2.13)$$

The third term is easily integrated since $P_{0,3}$ is constant with respect to t. Using the bounded function $\psi(s) = \sin(s/2)/s$ the integral reads

$$e^{-it(\sqrt{M(3k)}-3\omega_0)/2}t\psi(t(\sqrt{M(3k)}-3\omega_0))P_{0,3} - e^{it(\sqrt{M(3k)}+3\omega_0)/2}t\psi(t(\sqrt{M(3k)}+3\omega_0))P_{0,3}. \quad (2.14)$$

The first and second terms of (2.13) are bounded for all t in $H^1_\varepsilon(\mathbb{R})$ but the third is not. Indeed, for the second term one faces the function $\sin(tx)/x$ on the domain $x > 3k$ (since $M(3k) \geq 9k^2$) while for the third term the domain is $\mathbb{R}$. Thus, the second one is bounded by $1/3k$ while the third one grows like $t/2$. However, using the spatial decrease of $P_{0,3}$ we next show that the last term grows much slower.

For this we use the spectral representation theorem remarking that the spectrum of $M(s)$ for any $s \neq 0$ is described by (2.7) plus some eigenvalues. We prove

Lemma 2.15. *For $s \neq 0$ the following spectral decomposition holds*

$$M(s) = \sum_{j>0}\int_{-1/2}^{1/2}\lambda_j(s,\ell)p^c_j(s,\ell)d\ell + \sum_{l>0}\lambda^\flat_l(s)\mathcal{P}_l(s),$$

where $p^c_j(s,\ell)f(y) = e^{i\ell y}\left((e_j(s,\ell),\widetilde{f}(\ell,\cdot))_{\varepsilon_0}e_j(s,\ell,y) + p_j(s,\ell)f(y)\right)$ with p_j defined in the proof (Appendix B*) and $\widetilde{f}$ is the Bloch transform of f with respect to y. It is a spectral projector related to the essential spectrum of $M(s)$. The $\mathcal{P}_l(s)$ are finite dimensional spectral projectors related to the eigenvalues $\lambda^\flat_l(s)$ of $M(s)$.*

See Appendix B for the proof. The singular term in (2.14) thus reads:

$$t\psi(t(\sqrt{M(3k)}-3\omega_0)) = \sum_{j\geq 1}\int_{-1/2}^{1/2} t\psi(t(\sqrt{\lambda_j(3k,\ell)}-3\omega_0)p^c_j(3k,\ell)d\ell$$
$$+\sum_l t\psi(t(\sqrt{\lambda^\flat_l(3k)}-3\omega_0))\mathcal{P}_l(3k).$$

We remark that the only term which may be not bounded independently of t is the one of index j_0. For the other indexes one gets a bounded expression for all time $t \in [0, T/\eta^2]$. Moreover, thanks to Assumption 2.9 and third point of Lemma 2.5, $9\omega_0^2 \notin \{\lambda^\flat_l,\ l > 0\}$, so the discrete part is also integrable. The only problem is then for ℓ close to the values of $\pm\ell^0$ for which $9\omega_0^2 = \lambda_{j_0}(3k, \pm\ell^0)$. For those values one can use the stationary phase method thanks to Assumption 2.13. See Appendix C for the proof of the inequality. □

Remark 2.16. 1. *If Assumption* 2.13 *fails, i.e. $|\partial_\ell\lambda_j(\ell^0)| \leq \eta$ then the third harmonic hardly disperses. The growth of the energy is, according to Remark* 2.11 *linear in t. This means that this corrector becomes as big as A_1. The validity of the WKB approximation thus breaks down.*

2. *If Assumption* 2.9 *fails, $3\omega_0$ is resonant so one should add it in the expression of the leading term E_0. Since this harmonic does not interact with the fundamental mode, the PhC waveguide works as a bi-modal guide. However this case is unlikely to happen since the eigenvalues are not created according to a linear rule. More probably could $3\omega_0$ be "close" to an eigenvalue of $M(3k)$ thus developing a weak resonance in a similar fashion as in the previous point.*

2.3. Convergence

In this section we show that ηE_{app} with $E_{app} = \sum_{0\le j\le 2} \eta^j E_j$ is an approximate solution of (1.5) in the sense that it stays close to the exact solution of (1.5) with initial data $\eta(E_{app}(t=0), \partial_t E_{app}(t=0)) + \mathcal{O}(\eta^m)$ with m big enough. We will give the word "close" a clearer meaning by using the space $\mathcal{H}^s(T)$ (cf. definition (2.1)). Note that $E_{app}(t=0)$ only depends on the initial data $\mathcal{A}_0(T=0)$ and $\mathcal{A}_1(T=0)$. Indeed, we take $A_{2,1}(T=0)=0$ and $A_{2,3}(t=0)=0$ (in the weakly resonant case) since the second corrector does not bring any precision in Theorem 2.2 but it is needed for the convergence.

Let us thus study the residual between (1.5) and the equation solved by ηE_{app}. We set

$$\mathcal{R}(E) = (\partial_t^2 - \frac{1}{\varepsilon}\Delta)E + \begin{pmatrix} \partial_t^2 P \\ 0 \end{pmatrix}.$$

Formally $\mathcal{R}(\eta E_{app})$ is of order $\mathcal{O}(\eta^4)$ but in fact a little less when measured in the space $\mathcal{H}^s(T)$ (see Lemma 2.21).

Then we look for a solution of (1.5) under the form $E = \eta(E_{app} + \eta^n R)$. Plugging this expression into (1.5) we get

$$(\partial_t^2 - \frac{1}{\varepsilon}\Delta)R = -\eta^{2-n}\chi_3 \partial_t^2 \left((E_{app} + \eta^n R)^3 - E_{app}^3\right) + \eta^{-1-n}\mathcal{R}(\eta E_{app}). \tag{2.15}$$

We want to show the existence of a solution for this equation which survives for times of order $1/\eta^2$. Because of the nonlinearity we analyze the equation in a Sobolev algebra. Since ε is only piecewise continuous we have to be careful since we will need to estimate some differential commutators involving ε. One could consider the spaces defined by powers of $-\frac{1}{\varepsilon}\Delta$ but this requires a very precise description of the spectral representation of the operator and promises tedious calculations. Instead we use the fact that ε just depends on y so that we can use spaces with as many x-derivatives as we want. We thus use the spaces $H^{k,1}$ introduced in Definition (2.1).

Lemma 2.17. *For $k \ge 1$ we have*

$$H^{k,1}(\mathbb{R}^2) \subset L^\infty(\mathbb{R}, H^{k-1}(\mathbb{R})) \cap L^2(\mathbb{R}, W^{k-1,\infty}(\mathbb{R})),$$

where $W^{k,\infty}(\mathbb{R})$ is the space of functions defined in $\mathbb{R}$ whose kth derivative is bounded a.e. in $\mathbb{R}$. Moreover, if $k \ge 2$ then

$$H^{k,1}(\mathbb{R}^2) \subset H^1(\mathbb{R}, W^{k-2,\infty}(\mathbb{R})) \cap L^\infty(\mathbb{R}^2).$$

Proof. Indeed, setting $v = \partial_x^{k-1}u$ with $u \in C_0^\infty$ one has

$$\|v(\cdot,y)\|^2_{L^2(\mathbb{R})} = 2\int_{\mathbb{R}}\int_{-\infty}^{y} v(x,y)\partial_y v(x,y)dydx \le 2\|v\|_{L^2(\mathbb{R}^2)}\|\partial_y v\|_{L^2(\mathbb{R}^2)}.$$

Next, setting $v = \partial_y\partial_x^{k-2}u$ or $v = \partial_x^{k-1}u$ and using $\|v(\cdot,y)\|^2_{L^\infty} = \|v^2(\cdot,y)\|_{L^\infty}$ we find that

$$\int_{\mathbb{R}} \|v(\cdot,y)\|^2_{L^\infty(\mathbb{R})}dy \le 2\int_{\mathbb{R}}\int_{\mathbb{R}} |\partial_x v(x,y)v(x,y)|dxdy \le 2\|v\|_{L^2(\mathbb{R}^2)}\|v_x\|_{L^2(\mathbb{R}^2)}.$$

Finally, one has the identity $u^2 = \int_{-\infty}^{x}\int_{-\infty}^{y} \partial_x\partial_y u^2 dxdy$ from which we get

$$\|u\|^2_{L^\infty(\mathbb{R}^2)} \le 2\|\partial_x u\|_{L^2(\mathbb{R}^2)}\|\partial_y u\|_{L^2(\mathbb{R}^2)} + 2\|u\|_{L^2(\mathbb{R}^2)}\|\partial_x\partial_y u\|_{L^2(\mathbb{R}^2)} \le 4\|u\|_{H^{2,1}}.$$

One concludes the Lemma by density. □

Lemma 2.18. *For $s \ge 2$, the space $\mathcal{H}^s(T)$ is an algebra.*

Notations 2.19. *In the following $\partial_{x,t}^s$ will mean any combination $\partial_x^a\partial_t^b$ with $a+b=s$.*

Proof. We have to compute the L^2 norm of $\partial_{x,t}^s(ab)$ and $\partial_y\partial_{x,t}^{s-1}(ab)$. Let us focus on the second one. By Leibniz' rule, this term is a sum of terms like

$$T = (\partial_y^{\gamma_1}\partial_x^{\alpha_1}\partial_t^{\beta_1}a)\;(\partial_y^{\gamma_2}\partial_x^{\alpha_2}\partial_t^{\beta_2}b), \quad \sum_{j=1}^{2}\alpha_j + \beta_j + \gamma_j = s, \quad \gamma_1 + \gamma_2 = 1.$$

Let us take $\gamma_1 = 1$ and $\gamma_2 = 0$. First suppose $\alpha_1 + \beta_1 \leq s-2$ then from Lemma 2.17, the first term in T belongs to $L^2(\mathbb{R}; L^\infty(\mathbb{R}))$ and the second belongs to $L^\infty(\mathbb{R}; L^2(\mathbb{R}))$. Thus, the $L^2(\mathbb{R}^2)$ norm of T is bounded. Suppose now that $\alpha_1 + \beta_1 = s-1$ with $\gamma_1 = 1$, then $\alpha_2 + \beta_2 = 0$ so one uses that $b \in L^\infty(\mathbb{R}^2)$. ☐

The first step in proving the existence of a solution for (2.15) in $\mathcal{H}^s(T)$ requires a linear estimate for the equation which is needed to estimate the terms of an approximating sequence defined by Picard iterates. Because the equation is quasilinear we first need to incorporate the highest derivatives of the nonlinear term in the linear operator. The nonlinear term in (2.15) reads:

$$3E^2\partial_t^2 R + \eta^2\chi_3 N(E_{app}, \partial_t E_{app}, R, \partial_t R),$$

where N is a third degree polynomial function of its arguments. Inserting the first term in the linear operator yields

$$(1 + 3\eta^2\chi_3(E_{app} + \eta^n R)^2)\partial_t^2 R - \frac{1}{\varepsilon}\Delta R = \eta^2\chi_3 N(E_{app}, \partial_t E_{app}, R, \partial_t R) + \eta^{-1-n}\mathcal{R}(\eta E_{app}).$$

Setting $g = 1 + 3\eta^2\chi_3(E_{app} + \eta^n R)^2$ and $f = \eta^2\chi_3 N(E_{app}, \partial_t E_{app}, R, \partial_t R) + \eta^{-1-n}\mathcal{R}(\eta E_{app})$ equation (2.15) now reads

$$\varepsilon g \partial_t^2 R - \Delta R = \varepsilon f.$$

The associate energy is

$$\mathcal{F}(t) = \sqrt{\int_{\mathbb{R}^2} \varepsilon g |\partial_{x,t}^s \partial_t R|^2 + \|\partial_{x,t}^s \nabla R\|_2^2 \, dxdy}.$$

Lemma 2.20. *For all $s \in \mathbb{N}^*$, there is a polynomial function C such that the energy $\mathcal{F}(t)$ satisfies the differential inequality*

$$\frac{d}{dt}\mathcal{F}(t) \leq \|\partial_{x,t}^s f(t)\|_2 + \eta^2 C(\|R\|_\infty, \|E_{app}\|_\infty, \|\partial_{x,t}R\|_\infty, \|\partial_{x,t}E_{app}\|_\infty, \|\partial_{x,t}^{s+1}E_{app}\|_2)\mathcal{F}(t).$$

Proof. Apply $\partial_{x,t}^s$ to the equation, set $V = \partial_{x,t}^s R$, multiply the equation by $V_t = \partial_t V$ and integrate over $\mathbb{R}^2$. Using

$$\partial_{x,t}^s \varepsilon g \partial_t^2 R V_t = \varepsilon g V_{tt} V_t + \varepsilon[\partial_{x,t}^s, g]\partial_t^2 R V_t,$$

with $V_{tt} = \partial_t^2 V$ where $[a,b] = ab - ba$ we get

$$\frac{d}{2dt}\left(\int \varepsilon g |V_t|^2 + \|\nabla V\|_2^2\right) + \int \varepsilon[\partial_{x,t}^s, g]\partial_t^2 R V_t - \varepsilon \partial_t g |V_t|^2 = \int \varepsilon \partial_{x,t}^s f V_t$$

Setting $\mathcal{F}^2 = \int \varepsilon g |V_t|^2 + \|\nabla V\|_2^2$ and $c = \sup(\varepsilon/g)$ we get

$$\frac{d}{dt}\mathcal{F} \leq c(\|\partial_t g\|_\infty \mathcal{F} + \|[\partial_{x,t}^s, g]\partial_t^2 R\|_2 + \|\partial_{x,t}^s f\|_2)$$

We need to estimate the commutator. By the chain rule one can express $[\partial_{x,t}^s, g]\partial_t^2 R$ as a sum of terms like

$$\eta^{2+2n}(\partial_{x,t}^{m_1}R)(\partial_{x,t}^{m_2}R)(\partial_{x,t}^{m_3+2}R), \quad \text{or} \quad \eta^{2+n}(\partial_{x,t}^{m_1}E_{app})(\partial_{x,t}^{m_2}R)(\partial_{x,t}^{m_3+2}R),$$
$$\text{or} \quad \eta^2(\partial_{x,t}^{m_1}E_{app})(\partial_{x,t}^{m_2}E_{app})(\partial_{x,t}^{m_3+2}R).$$

with $m_1 + m_2 + m_3 \leq s$. We use the Hölder and Gagliardo-Nirenberg inequality to estimate the L^2 norm of those terms. Let us focus on the first one. First, for $m_j \leq 1$, $j \in \{1,2\}$ one can estimate directly the first product by

$$(\|R\|_\infty + \|\partial_{x,t}R\|_\infty)^2 \|\partial_{x,t}^{s+1}R\|_{L^2(\mathbb{R}^2)}.$$

Otherwise, setting $r = n + m_1 + m_2 - 1$, $p = r/(n+1)$, $q_1 = r/(m_1 - 1)$ and $q_2 = r/(m_2 - 1)$ the Hölder inequality leads for any given t, y in $[0,T] \times \mathbb{R}$

$$\|\partial_{x,t}^{m_1}R\partial_{x,t}^{m_2}R\partial_{x,t}^{n}\partial_t^2 R(t,.,y)\|_2 \leq \|\partial_{x,t}^{m_1}R(t,.,y)\|_{L^{2q_1}}\|\partial_{x,t}^{m_2}R(t,.,y)\|_{L^{2q_2}}\|\partial_{x,t}^{n+1}R_t(t,.,y)\|_{L^{2p}}.$$

Then, writing $\partial_{x,t}^{m_j} R = \partial_{x,t}^{m_j-1}\partial_{x,t} R$ and interpolating between $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$, the Gagliardo-Nirenberg inequality reads

$$\|\partial_{x,t}^{m_j} R(t,.,y)\|_{L^{2q_j}(\mathbb{R})} \leq C\|\partial_{x,t} R(t,.,y)\|_\infty^{1-1/q_j}\|\partial_{x,t}^{s+1} R(t,.,y)\|_2^{1/q_j}.$$

Finally, using the Hölder inequality, the L^2-norm in y of $\|\partial_{x,t}^{m_1} R\partial_{x,t}^{m_2} R\partial_{x,t}^{n}\partial_t^2 R(t,.,y)\|_2$ is bounded by

$$\|\partial_{x,t} R\|_{L^\infty(\mathbb{R}^2)}^2\|\partial_{x,t}^{s+1} R\|_{L^2(\mathbb{R}^2)}.$$

Doing the same with the other two terms we arrive at

$$\|[\partial_{x,t}^s, g]\partial_t^2 R\|_2 \leq \eta^2 C(\|R\|_\infty, \|E_{app}\|_\infty, \|\partial_{x,t} R\|_\infty, \|\partial_{x,t} E_{app}\|_\infty, \|\partial_{x,t}^{s+1} E_{app}\|_2)\mathcal{F},$$

from which the lemma follows. □

From the linear inequality we need to estimate $\|\partial_{x,t}^s f(t)\|_2$. Since we want to show the existence of a solution of Equation (1.5) on a time interval of size $\mathcal{O}(\eta^{-2})$ (diffractive time) we need to give estimates for such times. Let us begin with $\eta^{-1-n}\mathcal{R}(\eta E_{app})$. It is sufficient to estimate this term in $\mathcal{H}^s(T/\eta^2)$. According to the beginning of the present section one looks for an estimate in terms of $\mathcal{A}_0(T=0)$ and $\mathcal{A}_1(T=0)$.

Lemma 2.21. *There is a constant $C>0$ such that*

$$\|\mathcal{R}(\eta E_{app})\|_{\mathcal{H}^s(T/\eta^2)} \leq Cf(\eta)\eta^{4-1/2}\left(\|\mathcal{A}_0(T=0)\|_{H^{2s+2}(\mathbb{R})}^{2s+3} + \|\mathcal{A}_1(T=0)\|_{H^{2s+1}(\mathbb{R})}\right),$$

with $f(\eta)=1$ if $3\omega_0$ is non resonant and $f(\eta)=-\ln(\eta)$ if $3\omega_0$ is weakly resonant.

Proof. The terms involving $E_0, E_1, A_{2,1}$ and $A_{2,3}$ in the non resonant case are similar. We consider $A_{2,3}$ in the weakly resonant case separately.

First, consider for instance $A_{2,1}$. We need to estimate $\partial_{x,t}^s(1-\pi(k))A_{2,1}$ and $\partial_{x,t}^{s-1}\partial_y(1-\pi(k))A_{2,1}$ in $L^2(\mathbb{R}^2)$ for times $t\leq T/\eta^2$. We estimate the first using the expression (2.10) and the second making an energy estimate on (2.8), i.e. deriving the equation by $\partial_{x,t}^{s-1}$ and multiplying scalarly in $L_\varepsilon^2(\mathbb{R})$ by $\partial_{x,t}^{s-1}A_{2,1}$. From (2.10) one sees that the norms involve a sum of products of the kind $a(T,X)b(y)$ where b involves powers of the eigenvector w_0 and a powers of $\mathcal{A}_0$. We have

$$\sup_{\eta^2 t\leq T}\|a(\eta^2 t, \eta(x-vt))b(y)\|_{L^2(\mathbb{R}^2)} \leq \frac{\|b\|_2}{\eta^{1/2}}\sup_{\tau\leq T}\|a(\tau,.)\|_{L^2(\mathbb{R}_X)}.$$

There is a similar estimate for $\partial_{t,x}^s a(\eta^2 t, \eta(x-vt))$ in term of $\partial_{\tau,X}^s a$. Consider for instance $a=\mathcal{A}_0^3$. Since $\mathcal{A}_0$ solves the nonlinear Schrödinger equation (2.9) one can express $\partial_{\tau,X}^s a$ as a sum of finite products of $\partial_X^q\mathcal{A}_0$ where the total number of derivative is $2s+2$. Since $H^{2s+2}(\mathbb{R})$ is an algebra for $s\geq 0$ it is not difficult to show that $\partial_{\tau,X}^s\mathcal{A}_0^3$ is bounded in $L^2(\mathbb{R}_X)$ by the bound given in the lemma. For the other values of a the bound is even simpler.

Let us now consider $A_{2,3}$ when $3\omega_0$ is weakly resonant. Then $A_{2,3}$ is a sum of products $a(T,X)b(t,y)$ where a is as before and b is estimated according to Lemma 2.14. □

Theorem 2.22. *Let $s\geq 1$, choose $(\mathcal{A}_0,\mathcal{A}_1)\in H^{2s+2}(\mathbb{R})\times H^{2s+1}(\mathbb{R})$ and construct E_{app} as done in subsection 2.2. For all $\eta>0$ small enough, there exists a $T>0$ and a unique solution E of (1.5) with initial data $\eta(E_{app}(t=0),\partial_t E_{app}(t=0))+\mathcal{O}(\eta^{1+n})\in H^{s+1,1}\times H^{s,1}$ such that $E=\eta(E_{app}+f(\eta)\eta^{1/2}R)$ with f as in the previous lemma and $R\in\mathcal{H}^{s+1}(T/\eta^2)$.*

Proof. The proof of existence is done by using Picard iterates on equation (2.15) which we estimate in $\mathcal{H}^{s+1}(t)$ thanks to the linear estimate of lemma 2.20 and which converge for t small enough. The proof is quite standard in Sobolev algebra so we refer to [19].

Let us now show that the maximal time of existence is of order $\mathcal{O}(1/\eta^2)$. The proof depends on $3\omega_0$ but looks the same. We thus consider the weakly resonant case. Looking for E under the form

$\eta(E_{app} + f(\eta)\eta^{1/2}R)$ and using the linear differential estimate of Lemma 2.20 together with the fact that N is in the algebra $\mathcal{H}^{s+1}(T)$ we get

$$\frac{d}{dt}\mathcal{F}(t) \leq \eta^2 C\mathcal{F} - \frac{\ln(\eta)}{f(\eta)}\eta^{3-1/2-n}K(\|E_{app}(t)\|_\infty)\|\partial_{x,t}^{s+1}E_{app}(t)\|_2,$$

where C is the polynomial function of Lemma 2.20 and is a second order polynomials of

$$\|R(t)\|_\infty, \|\partial_{x,t}R(t)\|_\infty, \|E_{app}\|_\infty, \|\partial_{x,t}E_{app}\|_\infty, \|\partial_{x,t}^{s+1}E_{app}\|_2.$$

By Lemma 2.17 it follows that C is bounded by some smooth η-independent function $h(\mathcal{F}(t), \mathcal{F}_{app}(\eta^2 t))$ where $\mathcal{F}_{app}(T)$ is the energy of E_{app} in $\mathcal{H}^{s+1}(T)$. The function $\mathcal{F}_{app}$ just varies with T since the other variables are lost when taking the L^2 norm of E_{app}. The same works with $\|E_{app}(t)\|_\infty = h_1(\eta^2 t)$ and $\|\partial_{x,t}^{s+1}E_{app}(t)\|_2 = h_2(\eta^2 t)$. Making the change of variable $T = \eta^2 t$, $\widetilde{\mathcal{F}}(\eta^2 t) = \mathcal{F}(t)$ we get

$$\frac{d}{dT}\widetilde{\mathcal{F}}(T) \leq h(\widetilde{\mathcal{F}}(T), \mathcal{F}_{app}(T))\widetilde{\mathcal{F}}(T) - \frac{\ln(\eta)}{f(\eta)}\eta^{1/2-n}K(h_1(T))h_2(T).$$

Choosing $n = 1/2$ and $f(\eta) = -\ln(\eta)$ we conclude by Gronwall's lemma that $\widetilde{\mathcal{F}}$ is smaller than some function v solution of the ordinary differential equation. Since the latter does not depend on η we conclude that there exists some $T > 0$ such that $R \in \mathcal{H}^{s+1}(T/\eta^2)$. □

3. Conclusion and perspectives

We have shown for a specific class of 2d nonlinear PhC waveguides, periodic in one direction and homogeneous in the other, the existence of modulated pulses characterized by a parameter η, whose propagation is given by the nonlinear Schrödinger equation (2.9). The distance of propagation we describe is of order η^{-2}. For instance, if $\eta = 0.05$ and if we consider a PhC with periodicity 10^{-7}m we consider the propagation of waves on distances of order 10^{-4}m.

Harmonics of size of order η^2 are generated and stay localized in the waveguide or are radiating through the PhC according to the fact that the corresponding pulsation lies in a gap (non resonant case) or in a band (weakly resonant case) of the PhC spectrum. In the weakly resonant case the radiation is described by a transverse wave (dispersive) equation with moving source term localized where the main pulse is and which is responsible for a growth of the energy of the third harmonic like $\mathcal{O}(\log(t))$ for times $t \leq T/\eta^2$.

Since the leading term does not depend on the second corrector we see that the energy of the WKB solution may increase in the weakly resonant case. But this is allowed by the equation (1.5), for it describes just a part of the total system involving $U = (B_1, B_2, E_3)$. Thus E_3 may take some energy from B_1 and B_2.

Finally, we prove that if the solution of Equation (1.5) is close to the form of the WKB approximation at a given time then it stays $\eta^{3/2}$-close (in the non resonant case) or $-\ln(\eta)\eta^{3/2}$-close (in the weakly resonant case) to the latter in L^∞ norm for times of order η^{-2} and with $\alpha < 1/2$.

Let us now give some comments and perspectives.

1. The scattering problem.

   The analysis of the second corrector shows that the structure of the profile is not preserved (in comparison with the leading term). A perturbation method like the one used in [22] would be better adapted. One could indeed look for an exact solution of (1.5) under the form

   $$E(t, x, y) = f(t, x)\cos(\omega_0 t - k_0 x)w_0(y) + R(t, x, y),$$

   where $R(t, x, \cdot)$ is orthogonal to w_0. Such an Ansatz yields a wave equation for f with velocity $\|w_0\|_2$ coupled with the full equation for R through nonlinear terms. The equation for R looks like equation (2.12) in first approximation since the main driving term is the nonlinear term computed at f.

2. Removing Assumption 1.2.

   If we consider a PhC periodic in both directions we thus have to deal with
$$\varepsilon(x, y) = \varepsilon_0(x, y) + \tilde{\varepsilon}(x, y),$$
   with ε_0 periodic and $\tilde{\varepsilon}$ periodic in x with same periodicity and compactly supported in y. The operator M is now analyzed with the help of a Floquet-Bloch transform with respect to x. The resulting family of operators is $M(\ell_1) := -1/\varepsilon((\partial_x + i\ell_1)^2 + \partial_y^2)$, $\ell_1 \in [-1/2, 1/2[$ with domain $H^2_{per}([0, 2\pi] \times \mathbb{R})$ whose elements are 2π periodic in x.

   We expect that the items 1,2,4 and 5 of Lemma 2.5 still apply for $M(\ell_1)$. Making the assumption 2.6, the operator $M(\ell_1)$ possesses an eigenvalue whose eigenvector w_0 is periodic in x and exponentially decaying in y.

   Next, looking for a WKB approximate solution as presented here yields a leading term $E_0 = \mathcal{A}_0(T, X) w_0 e^{i(\omega t + \ell_1 x)} + c.c.$. The analysis of the first corrector remains the same but that of the second one changes. Indeed, the third equation involves the third harmonic which are not just exponentials but the cube of the Bloch mode $w_0(\cdot, y)e^{i\ell_1 \cdot}$. Moreover, the analysis of $E_{2,3}$ requires to perform the spectral resolution of M which is much more complicated since the solutions of the unperturbed homogeneous operator are not just as given in Lemma B.2 but are some convolution involving a Green kernel.

   Finally, the analysis of the convergence would be completely different since we used that ε is independent of x. The expected regularity is now finite with respect to x, y. We must find new algebra well suited for the operator M. We see three directions of investigation:

   - Using L^2 spaces of power of M i.e. spaces $\mathcal{E}^s$ defined by
$$\mathcal{E}^s = \left\{ u \in L^2(\mathbb{R}^2) \quad | \quad \|M^{a/2} u\|^2_\varepsilon < \infty, \quad \forall a \leq s \right\}.$$
   The space $\mathcal{E}^1$ is isomorphic to $H^1(\mathbb{R}^2)$ and $\mathcal{E}^2$ is isomorphic to $H^2(\mathbb{R}^2)$. Thus lemma 2.17 holds for $\mathcal{E}^2$. But we need to find a linear estimate like in Lemma 2.20. This requires to compute a commutator of the kind $[M^s, g]$ which seems difficult.

   - Using Strichartz estimates. Such estimates are naturally well-suited for operators with non smooth coefficients (see [20]).

   - Using local estimates on each cell of periodicity where the coefficients are smooth together with a global estimate in $L^2(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$. This should work for semilinear problems but is unclear for quasilinear problems.
3. Transverse magnetic waves. We refer to the vectorial equation written above Equation (1.5). The operator involved is $N = -\nabla \frac{1}{\varepsilon} \nabla$. It is self-adjoint in $L^2(\mathbb{R}^2)$ and enjoys similar properties as M (cf. [13]) but is more singular for non smooth ε. Moreover, if ε is as in the previous item, we do not know if any space of power of N is an algebra.
4. Non-straight waveguides. The main issue is to describe the spectrum of the underlying operator. A first problem consists in considering a half waveguide, i.e. $\tilde{\varepsilon}$ vanishing for $x > 0$. This is a reflection-transmission problem. It is interesting to compute how the transmitted wave radiates and if there are cases where total reflection happens.

   Next, in view of nano-circuits, one has to deal with waveguides making right angles (see [24]). Finally, it has been noticed (see [26]) that a slight local change of periodicity of the PhC near the defect row completely changes the propagation of light. We interpret this feature in terms of scattering as follows: if $\widetilde{M}$ refers to the operator of this structure, the slight local change of periodicity is a compact perturbation of the operator M which may provide $\widetilde{M}$ with an eigenvalue. Thus, when a wave polarized according to the guided mode comes around the perturbed region, a big part of the energy is transferred to the local mode which behaves as a defect for the guide thus scattering the incoming wave.

Appendix

A Proof of Lemma 2.5

Proof. 2) Next to see that $\sigma_{ess}M(k) = \sigma_{ess}M_0(k)$ we need to show that $(M(k)+1)^{-1} - (M_0(k)+1)^{-1}$ is compact according to a theorem of Weyl (cf. [30] Theorem 13.14, fourth Corollary). Using the factorization

$$(M(k)+1)^{-1}(M_0(k) - M(k))(M_0(k)+1)^{-1}$$

we show that $M_1(k) = (M_0(k) - M(k))(M(k)+1)^{-1}$ is bounded and that $M_2(k) = (M(k)+1)^{-1}\mathbb{1}_{\{\tilde{\varepsilon}\neq 0\}}$ is compact. Denoting by $\|\cdot\|$ the operator norm on L^2_ε and using

$$M(k) - M_0(k) = -\frac{\tilde{\varepsilon}}{\varepsilon_0}M(k), \quad \text{we get} \quad \|M_1(k)\| \leq c \quad \text{with} \quad c = \sup(\tilde{\varepsilon}/\varepsilon_0)^2.$$

Next, we show that $M_2(k)$ is an Hilbert Schmidt operator in $L^2_\varepsilon(\mathbb{R})$. First, because the norm $\|\cdot\|_\varepsilon$ is equivalent to $\|\cdot\|_{1/\varepsilon}$ it is sufficient to prove that $M_2(k)$ is an Hilbert Schmidt operator in $L^2_{1/\varepsilon}(\mathbb{R})$. But

$$(M_2(k)u, u)_{1/\varepsilon} = \int (-\Delta(k) + \varepsilon)^{-1}\mathbb{1}_{\{\tilde{\varepsilon}\neq 0\}}u\bar{u}.$$

So it is equivalent to show that $(-\Delta(k)+\varepsilon)^{-1}\mathbb{1}_{\{\tilde{\varepsilon}\neq 0\}}$ is Hilbert Schmidt in $L^2(\mathbb{R})$. Since the operator is self-adjoint in $L^2(\mathbb{R})$ and $(-\Delta(k)+\varepsilon) \geq (-\Delta(k)+\inf\varepsilon)$ it follows $(-\Delta(k)+\varepsilon)^{-1} \leq (-\Delta(k)+\inf\varepsilon)^{-1}$. So it is sufficient to prove that $\widetilde{M_2}(k) = (-\Delta(k) + \inf\varepsilon)^{-1}\mathbb{1}_{\{\tilde{\varepsilon}\neq 0\}}$ is Hilbert Schmidt in $L^2(\mathbb{R})$. Using the Fourier transform we can express the kernel of $\widetilde{M_2}(k)$ as follows

$$K_{\widetilde{M_2}}(k, y, y') = \frac{1}{2\pi}\int_{\mathbb{R}} e^{i\xi(y-y')}\frac{\mathbb{1}_{\{\tilde{\varepsilon}(y')\neq 0\}}}{k^2+\xi^2+1}d\xi.$$

It has a bounded $L^2(\mathbb{R}^2)$ norm (make two integrations by parts w.r.t. ξ).

3) The eigenvalues of $M(k)$ are points of the resolvent set of $M_0(k)$. This follows from the Floquet theorem. Indeed, suppose $\lambda \in \sigma_{ess}M_0(k)$ then there exists $j \in \mathbb{N}$ and $\ell \in [-1/2, 1/2)$ such that $\lambda = \lambda_j(\ell)$. The solutions of the ordinary differential equation (ODE) $(M(k) - \lambda)u = 0$ outside $[-a, a]$ are thus of the form $u(y) = p_1(y)e^{i\ell y} + p_2(y)e^{-i\ell y}$ with p_1, p_2 periodic if $\ell \notin \{0, 1/2\}$ and $u(y) = p_1(y) + p_2(y)y$ otherwise. In both cases $u \notin L^2(\mathbb{R})$.

Let us now show that the number of eigenvalues of $M(k)$ lying in the gap (λ_a, λ_b) of $M_0(k)$ is finite.

The proof goes along the lines of [18] using the Birman-Schwinger principle and a trace formula (also called Lieb-Thirring formula). However, since the domain of $M(k)$ depends on the weight ε we need to adapt the developments found in the above quotation. For sake of self consistency we recall those developments in our setting. We use Assumption 2.6 and first suppose that $\tilde{\varepsilon} < 0$. Let λ be an eigenvalue of $M(k)$ in a gap (λ_a, λ_b) of $M_0(k)$. The eigenvalue problem reads:

$$M(k)u = \lambda u \Leftrightarrow \frac{\varepsilon_0}{\varepsilon}(M_0(k) - \lambda)u = (1 - \frac{\varepsilon_0}{\varepsilon})u \Leftrightarrow u = R_0(\lambda)\frac{\tilde{\varepsilon}}{\varepsilon_0}u.$$

Since $\tilde{\varepsilon} < 0$ let us set $V = \sqrt{-\tilde{\varepsilon}/\varepsilon_0}$ and $v = Vu$. We have

$$v = -VR_0(\lambda)Vv = K(\lambda)v.$$

First, doing as in step 2) one shows that $K(\lambda)$ is compact. Let us denote by $\mu_1 > \mu_2 > \ldots > 0$ its positive eigenvalues. Next, note that $R_0(\lambda)$ is increasing with λ. Thus $K(\lambda)$ is decreasing. From this and the minimax principle one deduces that the eigenvalues of $K(\lambda)$ are decreasing. For $s > 0$ smaller than $\lambda_b - \lambda_a$, let $N(\lambda_a + s, \lambda_b)$ be the number of eigenvalues of $M(k)$ situated in the gap $(\lambda_a + s, \lambda_b)$. Each eigenvalue λ_j corresponds to a μ_l such that $\mu_l(\lambda_j) = 1$. From the decrease of the μ_l we see that λ_a is the unique possible accumulating point for the λ_j. We next check if it is the case by estimating $N(\lambda_a + s, \lambda_b)$ when s goes to zero. Calling $Tr(A)$ the trace of a Hilbert-Schmidt operator A we have

$$N(\lambda_a + s, \lambda_b) \leq \text{Card}\{\mu_j(\lambda_a + s) \geq 1\} \leq \text{Tr}(\widetilde{K}(\lambda_a + s)^{2\theta}), \quad \forall\theta \geq 0.$$

The operator $\widetilde{K}(\lambda)$ is defined by the restriction of $K(\lambda)$ to the subspace $\mathcal{E}$ where it is bigger than 1. So, on $V\mathcal{E}$ there holds $-R_0(\lambda) \geq 1$. Thanks to the Bloch transform one sees that this resolvent has a band-gap spectrum described by

$$\bigcup_{j>0,\ \ell\in[-1/2,1/2)} \frac{1}{\lambda-\lambda_j(\ell)}.$$

One thus needs to consider those j for which $\lambda_a + s > \lambda_j(\ell),\ j < j_0$ where j_0 is such that λ_a belongs to λ_{j_0}. Denoting by $-\widetilde{R}_0(\lambda)$ the corresponding operator we have $\widetilde{K}(\lambda) = -V\widetilde{R}_0(\lambda)V$. Next for any $\theta > 0$, Jensen inequality implies

$$(\widetilde{K}(\lambda)u,u)^\theta \leq (\widetilde{K}^\theta(\lambda)u,u),$$

thus, using the minimax principle as in [[17],Lemma 21] we get

$$\mu_j^{2\theta}(\lambda) \leq \mu_j(\theta,\lambda)^2$$

where $\mu_j(\theta,\lambda)$ are the eigenvalues of the operator $-V\widetilde{R}_0^\theta(\lambda)V$. Thus

$$N(\lambda_a+s,\lambda_b) \leq \operatorname{Tr}\left((V\widetilde{R}_0^\theta(\lambda)V)^2\right).$$

The last quantity is bounded by the L^2-norm of the kernel W of $-V\widetilde{R}_0^\theta(\lambda)V$. Using the Bloch transform we get

$$W(x,y) = V(x)V(y)\sum_{j\leq j_0,k}\int_{-1/2}^{1/2} e^{i\ell x}e^{-i(k+\ell)y}(e^{ik\cdot},e_j(\ell))(\lambda_j(\ell)-\lambda)^{-\theta})e_j(\ell,x)d\ell.$$

First, gathering the terms with index k yields $\sum_k e^{-iky}(e^{ik\cdot},e_j(\ell)) = \overline{e_j(\ell,y)}$. Then letting $c_{j_1,j_2}(\ell_1,\ell_2) = \int_{\mathbb{R}} V^2(y)e_{j_1}(\ell_1,y)\overline{e_{j_2}}(\ell_2,y)dy$ we have

$$\|W\|^2_{L^2(\mathbb{R}^2)} = \iint_{-1/2}^{1/2} e^{i(\ell_1-\ell_2)(x-y)}\sum_{j_1\leq j_0,\,j_2\leq j_0}\int |c_{j_1,j_2}(\ell_1,\ell_2)|^2(\lambda_{j_1}(\ell_1)-\lambda)^{-\theta}(\lambda_{j_2}(\ell_2)-\lambda)^{-\theta}d\ell_1 d\ell_2.$$

The numbers $c_{j_1,j_2}(\ell_1,\ell_2)$ are bounded by $p\|V\|^2_\infty$ where p is the smallest number such that $p\pi >$ supp$\tilde{\varepsilon}$. We thus have

$$\|W\|_{L^2(\mathbb{R}^2)} \leq p\|V\|^2_\infty\left(\int_{-1/2}^{1/2}\sum_{j\leq j_0}\left|(\lambda_j(\ell)-\lambda)^{-\theta}\right|d\ell\right)^{1/2}.$$

Now let us consider j such that $\sup_\ell \lambda_j(\ell) - \lambda = s$. Assuming that the supremum is reached for $\ell = 0$ we get $\lambda_j(\ell) = \lambda_j(0) + c_j\ell^2 + \mathcal{O}(\ell^3)$ where $c_j = \lambda_j''(0)$ is assumed to be non zero and $\lambda_j(0) = \lambda_a$. Then, for $\alpha > 0$ small but independent of s we have

$$\int_{-\alpha}^{\alpha}(\lambda_j(\ell)-\lambda)^{-\theta}d\ell = \int_{-\alpha}^{\alpha}(s+c_j\ell^2)^{-\theta})d\ell = s^{1/2-\theta}\int_{-\alpha/\sqrt{s}}^{\alpha/\sqrt{s}}(1+c_j\ell^2)^{-\theta}d\ell.$$

When $\theta < 1/2$ the last integral is equivalent to $s^{-1/2+\theta}$ and the whole quantity is bounded.

Remark A.1. *If $c_j = 0$ then the last integral still converges if we take $\theta < 1/(n+1)$ where n is the order of degeneracy of λ_j at 0.*

If $\tilde{\varepsilon} > 0$, K would be increasing. The possible accumulation point is thus λ_b and one has

$$N(\lambda_a,\lambda_b-s) \leq Card\{\mu_j(\lambda_b-s)\geq 1\}.$$

The previous analysis then holds, taking into account those changes.

4) We refer to [15], Theorem 2. The main idea is a scaling used together with the formula

$$dist(\lambda,\sigma(M(k))) = \inf_{\varphi,\|\varphi\|_2=1}\|(M(k)-\lambda)\varphi\|_2$$

where $\sigma(M(k))$ is the spectrum of $M(k)$. One looks for $\lambda \in (\lambda_a, \lambda_b)$ and for a φ with norm 1 and support in supp$\tilde{\varepsilon}$ such that

$$\|(M(k)-\lambda)\varphi\|_2 < \max_{i=a,b}(|\lambda-\lambda_i|).$$

5) The regularity of the eigenfunction is immediate. To complete the proof we must show the exponential decay of the eigenfunction. This is a general fact for isolated eigenvalues (see [1] and the review [2]). Here, in 1d, one can easily check this fact. Indeed, the eigenfunction w_0 solves the second order ODE $(M_0(k)-\omega_0^2)w_0 = 0$ with periodic coefficients out of the interval $[-a,a]$. Because ω_0^2 is in a spectral gap of $M_0(k)$, the associated Floquet exponents $\pm\ell_0$ are imaginary (see the proof of lemma 2.12). Therefore w_0 decays exponentially like $e^{-|\ell_0 y|}$.

□

B Proof of Lemma 2.15

The proof is quite long so we formulate intermediate lemmas to gather the results. We first compute the resolvent of $M(k)$ (cf. Lemma B.1) and then we compute the spectral projector (cf. Lemma B.5). First note that $M(k) \geq k^2$ in $L^2_\varepsilon(\mathbb{R})$. This allows to use Stone's Formula to compute the spectral projectors for $M(k)$:

$$M(k) = \int_{k^2}^{\infty} \lambda dE_\lambda, \quad E_\lambda = \frac{1}{2i\pi}\lim_{\nu\to 0}\int_0^\lambda (M(k)-\mu-i\nu)^{-1} - (M(k)-\mu+i\nu)^{-1}d\mu.$$

The last formula holds for any $\lambda \notin \sigma_p(M(k))$ (point spectrum). For such λs we thus have

$$dE_\lambda = \frac{1}{2i\pi}\lim_{\nu\to 0}(R_{\lambda+i\nu} - R_{\lambda-i\nu}), \qquad \text{with } R_{\lambda+i\nu} = (M(k)-\lambda-i\nu)^{-1}. \tag{B.1}$$

We thus need to compute the resolvent $R_z,\ z = \lambda + i\nu$.

Lemma B.1. *For $z \in ResM(k)$ we have $R_z = R_{0z} + \widetilde{R}_z$ where R_{0z} is the resolvent of the unperturbed operator $M_0(k)$*

$$R_{0z}f = \int_{-1/2}^{1/2} e^{iy\ell}\sum_{j>0}\frac{f_j}{\lambda_j(k,\ell)-z}e_j(\ell)d\ell,$$

and

$$\widetilde{R}_z f = \begin{cases} c_-(z)e_m(y)e^{k_-(z)y}, & y < -a \\ c_-(z)r(z,y)e^{-ak_-(z)}, & y \in [-a,a] \\ c_+(z)\bar{e}_m(y)e^{k_+(z)y}, & y > a \end{cases}$$

The scalars $c_\pm(z)$ are defined in the proof and depend on f. The scalar function r and the scalars $k_\pm(z)$ are also computed in the proof and do not depend on f (it just depends on the solution of the ODE $(M(k)-z)u = 0$).

Proof. Let us consider the equation

$$(M(k)-z)u = f \quad \text{in} \quad L^2_\varepsilon(\mathbb{R}).$$

Let us look for $u = U + r$ where U is computed through the unperturbed operator $M_0(k)$.

$$(M_0(k)-z)U = f \quad \text{and} \quad (M(k)-z)r = \frac{\tilde{\varepsilon}}{\varepsilon}(f+zU).$$

1. The first equation is handled with the Floquet-Bloch theorem. Indeed, applying the Floquet-Bloch transform we get for all $\ell \in [-1/2, 1/2)$

$$(M_0(k,\ell)-z)\widetilde{U}(y,\ell) = \widetilde{f}(y,\ell), \quad \text{in} \quad L^2([0,2\pi]).$$

We use the notation of Appendix A, 1. Since

$$z \notin \sigma(M(k)) \supset \sigma(M_0(k)) = \bigcup_{j>0} \{\lambda_j(k,\ell), \quad \ell \in [-1/2, 1/2]\},$$

one can solve the equation. Writing $U = \sum_{j>0} U_j e_j$ and setting $f_j(\ell) = (e_j(\ell), \widetilde{f})_{\varepsilon_0}$ we get

$$U(z) = \int_{-1/2}^{1/2} e^{iy\ell} \sum_{j>0} \frac{f_j(\ell)}{\lambda_j(k,\ell) - z} e_j(\ell) d\ell. \tag{B.2}$$

2. Now, considering the equation for r let us note that for all y such that $\tilde{\varepsilon} = 0$ (i.e. $|y| > a$) one has

$$(M_0(k) - z)\, r(y) = 0, \quad \text{i.e.} \quad -\partial_y^2 r + k^2 r - z\varepsilon_0(y) r = 0. \tag{B.3}$$

Because z is in the resolvent set of $M_0(k)$ we have

Lemma B.2. *The differential equation* (B.3) *possesses two solutions r_-, r_+ with the following property:*

$$r_\pm(y) = q_\pm(z,y) e^{\zeta_\pm(z) y}, \quad \Re(\zeta_-(z)) > 0, \quad \zeta_+(z) = -\zeta_-(z).$$

where $q_\pm(z,\cdot)$ are 2π periodic.

Proof. The general solutions of the equation are given by the Floquet theorem and look like $q(y)e^{\zeta y}$ with q periodic and $\Im\zeta \in [-1/2, 1/2)$ or $yq(y)$ (when $\zeta = 0$). Then $\Re(\zeta) \neq 0$ since otherwise z would be in the essential spectrum of $M_0(k)$.

To see that $\zeta_- = -\zeta_+$ one has to consider the so-called discriminant equation (cf. Eastham [12]) which allows to determine ζ_+, ζ_-. We recall it quickly. First define the fundamental 2×2 matrix $Q_0(y)$ solution of the equation and with identity initial value. The eigenvalues $\rho_\pm$ of Q_0 are related to the $\zeta_\pm$ by $\rho_\pm = e^{2\pi\zeta_\pm}$ (see Eastham [12]). They are solution of $\rho^2 - (\mathrm{tr} Q_0(2\pi))\rho + 1 = 0$. There are two solutions satisfying $\rho_+\rho_- = 1$, which is equivalent to $\zeta_- = -\zeta_+$ modulo i. $\square$

Notations B.3. *In the following we fix the choice of $q_-(z), q_+(z)$ by*

$$\|q_-(z)\|_{L^2(0,2\pi)} = \|q_+(z)\|_{L^2(0,2\pi)} = 1,$$

and we write

$$r_\pm(y) = c_\pm(z) q_\pm(z,y) e^{\zeta_\pm(z) y}, \quad \pm y > a \tag{B.4}$$

where $c_-(z), c_+(z)$ are complex numbers.

Since we look for u in the image of $L^2(\mathbb{R})$ by the resolvent of $M(k) - z$ one must check that $u \in H^2(\mathbb{R}) \subset C^1(\mathbb{R})$. So, for $y \in [-a, a]$ the equation for r

$$(M(k) - z) r = \frac{\tilde{\varepsilon}}{\varepsilon}(f + zU),$$

has to be solved together with the boundary conditions

$$R_\pm(\pm a) = \begin{pmatrix} r_\pm(\pm a) \\ r'_\pm(\pm a) \end{pmatrix} = c_\pm(z) \begin{pmatrix} q_\pm(z, \pm a) \\ q'_\pm(z, \pm a) + \zeta_\pm(z) q_\pm(z, \pm a) \end{pmatrix} e^{\pm a\zeta_\pm(z)}.$$

We define $\widetilde{R}_\pm(\pm a)$ such that $R_\pm(\pm a) = c_\pm(z)\widetilde{R}_\pm(\pm a)$. Those boundary conditions can be also considered as one initial data at $\pm a$ plus an extra boundary condition at $\mp a$. Let us solve the equation as an initial value problem at $-a$. First remark that $\widetilde{R}_-(-a) \neq 0$ for all values of z since otherwise, because of the Cauchy theorem the solution of $(M(k) - z)r = 0$ on $(-\infty, a]$ would vanish (the same holds for $\widetilde{R}_+(a)$). Let us use the variation of constant formula and call $Q(z)$ the fundamental matrix of the equation:

$$\partial_y Q(z,y) = A(z,y) Q(z,y), \quad y \in [-a, a], \quad A(z,y) = \begin{pmatrix} 0 & 1 \\ k^2 - z\varepsilon & 0 \end{pmatrix}, \quad Q(z, -a) = Id.$$

Then the solution $R = (r, r')$ of the equation is given by

$$R(y) = Q(z,y) R_-(-a) + Q(z,y) \int_{-a}^{y} Q^{-1}(z,s) F(s) ds, \quad F = \begin{pmatrix} 0 \\ \frac{\tilde{\varepsilon}}{\varepsilon}(f + zU) \end{pmatrix}. \tag{B.5}$$

Next the boundary condition at a gives the equation

$$Q(z,a)R_-(-a)+Q(z,a)\int_{-a}^{a}Q^{-1}(z,s)F(s)ds=R_+(a).$$

We thus have two equations with two unknown $(c_-(z),c_+(z))$. This problem has a unique solution if and only if $Q(z,a)\widetilde{R}_-(-a)$ and $\widetilde{R}_+(a)$ are not collinear. In this case, noting $P(z)=[-Q(z,a)\widetilde{R}_-(-a),\widetilde{R}_+(a)]$ (2×2 matrix with column vectors $-Q(z,a)\widetilde{R}_-(-a)$ and $\widetilde{R}_+(a)$) we get

$$\begin{pmatrix}c_-(z)\\ c_+(z)\end{pmatrix}=P^{-1}(z)Q(z,a)\int_{-a}^{a}Q^{-1}(z,s)F(s)ds. \tag{B.6}$$

□

Lemma B.4. *P is holomorphic and the zeros of $det(P)$ are the eigenvalues of $M(k)$.*

Proof. The matrix $Q(\cdot,a)$ is holomorphic since it is solution of $Q'=AQ$ where A is an holomorphic matrix and $\widetilde{R}_\pm(\pm a)$ are holomorphic for the same reasons. Thus P is holomorphic.

Next suppose that $\det P=0$. The relation $Q(z,a)R_-(-a)=R_+(a)$ will be satisfied for a value of $c_-(z)/c_+(z)\in\mathbb{R}^*$. Then, the functions u defined by (B.4) and (B.5) are solution of $(M(k)-z)u=0$. Reciprocally, if λ is an eigenvalue of $M(k)$, then any eigenvector w satisfies the equation on $[-a,a]$ with the boundary conditions and thus satisfies $Q(z,a)R_-(-a)=R_+(a)$ where $R_\pm$ are constructed as above with w instead of r. □

We now compute the spectral projector by using Stone's formula (B.1).

Lemma B.5. *For $\lambda=\lambda_{j_0}(k,\ell)$ the spectral projector can be expressed as follows:*

$$dE_\lambda=\left(e^{i\ell y}p^c_{j_0}(k,\ell)+e^{-i\ell y}p^c_{j_0}(k,-\ell)\right)d\ell,\quad \ell\in[0,1/2]$$

where

$$p^c_j(k,\ell)f=p_j(k,\ell)f+(\widetilde{f},e_j(k,\ell))_{\varepsilon_0}e_j(k,\ell),$$

with

$$p_j(k,\ell)f=\begin{cases} c_-(\lambda_j(k,\ell))\partial_\ell\lambda_j(k,\ell)e_j(k,\ell,y), & y<-a,\\ c_-(\lambda_j(k,\ell))\partial_\ell\lambda_j(k,\ell)r(\lambda_j(k,\ell),y)e^{-i\ell(a+y)}, & y\in[-a,a],\\ c_+(\lambda_j(k,\ell))\partial_\ell\lambda_j(k,\ell)e_j(k,\ell,y), & y>a,\end{cases}$$

where r is the first component of the vector R given by (B.5).
For $\lambda\in\mathbb{R}^+\setminus\bigcup_j Im\lambda_j(k)$

$$dE_\lambda=\sum_l\mathcal{P}_l(k)\delta(\lambda^\flat_l,\lambda)d\lambda,$$

where $\delta(\lambda^\flat_l)$ is the Dirac function centered at the eigenvalue $\lambda^\flat_l$ and

$$\mathcal{P}_l(k)=\frac{1}{2i\pi}\int_{B(\lambda^\flat_l)}(M(k)-z)^{-1}dz,$$

where $B(\lambda^\flat_l)$ is a small ball around $\lambda^\flat_l$ containing just $\lambda^\flat_l$.

Proof. **1**. The contribution of the unperturbed operator is

$$\frac{1}{2i\pi}\lim_{\nu\to 0}U_{\lambda+i\nu}-U_{\lambda-i\nu}=\frac{1}{\pi}\lim_{\nu\to 0}\int_{-1/2}^{1/2}f_j(\ell)e_j(\ell)e^{iy\ell}\frac{\nu}{(\lambda_j(k,\ell)-\lambda)^2+\nu^2}d\ell.$$

The index j is such that $\lambda \in \mathrm{Im}\lambda_j$. Obviously if λ is in a gap then the limit vanishes. Let $\pm\ell^\lambda$ be the solutions of the equation $\lambda = \lambda_j(\ell)$. Then, splitting the integral and making a change of variable in each bit yields

$$\frac{1}{2i\pi}\lim_{\nu\to 0} U_{\lambda+i\nu} - U_{\lambda-i\nu} = \frac{1}{\partial_\ell\lambda_j(-\ell^\lambda)} f_j(-\ell^\lambda)e_j(-\ell^\lambda)e^{-iy\ell^\lambda} + \frac{1}{\partial_\ell\lambda_j(\ell^\lambda)} f_j(\ell^\lambda)e_j(\ell^\lambda)e^{iy\ell^\lambda}.$$

Finally, using that $d\lambda = \partial_\ell\lambda_j(\ell^\lambda)d\ell^\lambda$ yields the expression of dE_λ given in the lemma.

2. Now the limit $\lim_{\nu\to 0} r(\lambda+i\nu) - r(\lambda-i\nu)$ depends on that λ is in the essential spectrum of $M(k)$ or an eigenvalue.

First case: $\lambda \in \sigma_{ess}(M(k))$.
By Lemma 2.5, 2., $\lambda = \lambda_j(\ell)$ for some j and ℓ. We have

$$\lim_{\nu\to 0} q_-(\lambda+i\nu) = c_-(\lambda)e_m(\ell) \quad \text{and} \quad \lim_{\nu\to 0} \zeta_-(\lambda+i\nu) = i\ell.$$

For $z = \lambda - i\nu$ the previous limits are changed into their complex conjugate. We thus have

$$\frac{1}{2i}\lim_{\nu\to 0} r_-(\lambda+i\nu) - r_-(\lambda-i\nu) = \Im\left(c_-(\lambda)e_m(y)e^{i\ell y}\right), \quad y < -a.$$

Then from Lemma B.2 one gets $\lim_{\nu\to 0} q_+(\lambda+i\nu) = \bar{c}_+(\lambda)\bar{e}_m(\ell)$ and $\lim_{\nu\to 0} \zeta_+(\lambda+i\nu) = -i\ell$. Thus

$$\frac{1}{2i}\lim_{\nu\to 0} r_+(\lambda+i\nu) - r_+(\lambda-i\nu) = -\Im\left(c_+(\lambda)e_m(y)e^{i\ell y}\right), \quad y > a.$$

Next for $r(y)$, $y \in [-a,a]$ we need to take the limit of the expression (B.6) as ν goes to zero. The functions P and $Q(\cdot,a)$ are holomorphic and non vanishing on a neighborhood of $\lambda = \lambda_j(\ell)$ (for all values of ℓ) thanks to Lemma 2.5, 3) and Lemma B.4. Thus P^{-1}, Q^{-1} are holomorphic on a neighborhood of λ. Hence the validity of the formula

$$\lim_{\nu\to 0} r(\lambda+i\nu) - r(\lambda-i\nu) = \Im\left(c_-(\lambda)r(\lambda,y)e^{-i\ell a}\right), \quad y \in [-a,a].$$

Second case: $\lambda \in \sigma_p(M(k))$.
From Lemma 2.5 one knows that λ is in a gap and that it is away from the remaining spectrum. So, according to Theorem 6.17 [23] one can express the projector by using the simpler formula:

$$\mathcal{P}_l(k) = \frac{1}{2i\pi}\int_{B(\lambda_l^\flat)} R_z dz,$$

where $B(\lambda_l^\flat)$ is a small ball around $\lambda_l^\flat$ containing the single eigenvalue $\lambda_l^\flat$.

□

C Proof of Lemma 2.14

Here we prove the inequality of the quoted Lemma:

$$\|\partial_t^{s+1}A_{2,3}\|_\varepsilon + \|\partial_t^s\partial_y A_{2,3}\|_\varepsilon \le c(1+\ln(t))\|(1+|y|)^2 P_{0,3}\|_\varepsilon.$$

Proof. Let us first take $s = 0$. The case $s > 0$ is obtained by doing the same analysis after differentiating the equation (2.12) s times in time and it is simpler since the right hand side vanishes. So it is sufficient to focus on the last term of $A_{2,3}$ in (2.13) and in particular on:

$$\widetilde{A}_{2,3} = t\psi(t(3\omega_0 - \sqrt{M(3k)}))P_{0,3},$$

where we recall that $\psi(t) = \sin(t/2)/t$. Since ψ is well defined on the spectrum of $\omega_0 - \sqrt{M(3k)}$ and continuous, the quantity $t\psi(t(3\omega_0 - \sqrt{M(3k)}))$ thus defines a self-adjoint operator. Thus we have

$$\left\|\widetilde{A}_{2,3}\right\|_\varepsilon^2 = \left(t^2\psi(t(3\omega_0 - \sqrt{M(3k)}))^2 P_{0,3}, P_{0,3}\right)_\varepsilon.$$

Using the spectral decomposition of $M(3k)$ we get:

$$\left\|\widetilde{A}_{2,3}\right\|_\varepsilon^2 = \sum_{j\geq 0}\int_{-1/2}^{1/2} t^2\psi^2(t(3\omega_0 - \sqrt{\lambda_j(3k,\ell)}))(p_j^c(3k,\ell)P_{0,3},P_{0,3})_\varepsilon d\ell$$
$$+\sum_{l\geq 0} t^2\psi^2(t(3\omega_0-\sqrt{\lambda_l^\flat(3k)}))(\mathcal{P}_l(3k)P_{0,3},P_{0,3})_\varepsilon.$$

Taking up the notations used in the hint of proof there are a ℓ^0 and a j_0 such that $\sqrt{\lambda_{j_0}(\pm\ell^0)} = 3\omega_0$. From Assumption 2.13, $\partial_\ell\lambda_{j_0}(\ell^0)\neq 0$. Let $[\alpha,\beta]$ be a neighborhood of ℓ^0 on which the derivative of λ_{j_0} does not vanish and let I be $\mathrm{Im}\sqrt{\lambda_{j_0}}([\alpha,\beta])$. We thus split the expression for $|\widetilde{A}_{2,3}\|_\varepsilon^2$ into two terms, T_1 and T_2 where

$$T_1 = \int_\alpha^\beta t^2\psi^2(t(3\omega_0-\sqrt{\lambda_{j_0}(3k,\ell)}))(p_{j_0}^c(3k,\ell)P_{0,3},P_{0,3})_\varepsilon d\ell \quad\text{and}\quad T_2 = \left\|\widetilde{A}_{2,3}\right\|_\varepsilon^2 - T_1.$$

Let us first estimate T_2. The function g defined by $g(x) = \mathbb{1}_{\{x\notin I\}}t^2\psi^2(t(3\omega_0-x))$ is bounded independently of t by $\mathbb{1}_{\{x\notin I\}}/(3\omega_0-x)^2$. Thus, setting $\varphi(\ell) = 3\omega_0-\sqrt{\lambda_{j_0}(\ell)}$ we have

$$T_2 = (g(M(3k))P_{0,3},P_{0,3})_\varepsilon \leq \max(|\varphi(\alpha)|^{-2},|\varphi(\beta)|^{-2})\|P_{0,3}\|_\varepsilon^2.$$

As for T_1 we use the exponential decay of $P_{0,3}$, i.e. the regularity of the quantity $(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon$ w.r.t. ℓ. Let G be a primitive of ψ^2 which vanishes at infinity. Since $t^2\psi^2$ is even it is sufficient to consider the integral on $[\ell^0,\beta]$. Now, integrating by parts between $[\ell^0,\beta]$ yields

$$T_1 = \left[tG(t\varphi(\ell))\frac{(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon}{\partial_\ell\varphi(\ell)}\right]_{\ell^0}^\beta - \int_{\ell^0}^\beta tG(t\varphi(\ell))\partial_\ell\frac{(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon}{\partial_\ell\varphi(\ell)}d\ell.$$

Since $\sin(x)\leq\min(1,x)$ for $x>0$, one finds that $G(x)$ is bounded by $1-x/4$ for $0\leq x\leq 2$ and $1/x$ for $x>2$. Thus, for t big enough the quantity between brackets is bounded by some constant times $\max(|\partial_\ell\varphi(\beta)|^{-1},|\partial_\ell\varphi(\ell_0)|^{-1})$. Then, the integral is bounded by

$$\sup_{\ell\in[\alpha,\beta]}\partial_\ell\frac{(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon}{\partial_\ell\varphi(\ell)}\int_{\ell^0}^\beta tG(t\varphi(\ell))d\ell$$

Making the change of variable $\tau=\varphi(\ell)$ the last integral can be estimated by

$$\sup_{\ell\in[\ell^0,\beta]}(\partial_\ell\varphi(\ell))^{-1}\int_0^r tG(t\tau)d\tau.$$

The last integral also reads $\int_0^{tr}G(y)dy$ which is bounded by $3+2\ln(tr/2)$. The same holds on $[\alpha,\ell^0]$.

Now we need to estimate all the constants coming in front of the integral, namely $\partial_\ell^m(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon$ and $\partial_\ell^m\lambda_{j_0}$ uniformly w.r.t. $\ell\in[\alpha,\beta]$ and $m\in\{0,1\}$. Recalling that $p_{j_0}^c = e^{i\ell y}(p_{j_0}+(e_{j_0},\widetilde{\cdot})_{\varepsilon_0}e_{j_0})$ and setting $D_\ell(y)=\partial_\ell+iy$ we get

$$\partial_\ell(p_{j_0}^c P_{0,3},P_{0,3})_\varepsilon = e^{i\ell y}\left(D_\ell(y)p_{j_0}P_{0,3},P_{0,3}\right)_\varepsilon + e^{i\ell y}\sum(D_\ell^{a'}(y)e_{j_0},D_\ell^{b'}(y)\widetilde{P}_{0,3}(\ell))_{\varepsilon_0}(D_\ell^{c'}(y)e_{j_0},P_{0,3})_\varepsilon,$$

where $a',b',c'\in\{0,1\}$ and $a'+b'+c'=1$. Let us begin by estimating the derivative of the scalar products in the sum.

1. Estimating $(D_\ell^{c'}(y)e_{j_0},P_{0,3})_\varepsilon$.

$$(D_\ell^{c'}(y)e_{j_0},P_{0,3})_\varepsilon \leq \|e_{j_0}\|_\infty\|y\varepsilon P_{0,3}\|_{L^1(\mathbb{R})} + \|\partial_\ell e_{j_0}\|_\infty\|\varepsilon P_{0,3}\|_{L^1(\mathbb{R})}.$$

The sup norm of e_{j_0} and $\partial_\ell e_{j_0}$ is estimated by the $L^2([0,2\pi])$ norm of their derivative w.r.t. y. Using the definition of $M_0(3k,\ell)$ one easily finds :

$$\|(\partial_y + i\ell)\partial_\ell^p e_{j_0}\|^2_{L^2([0,2\pi])} = (M_0(3k,\ell)\partial_\ell^p e_{j_0}, \partial_\ell^p e_{j_0})_{\varepsilon_0} - 9k^2\|\partial_\ell^p e_{j_0}\|_{L^2([0,2\pi])}$$
$$= \lambda_{j_0}(\ell)\|\partial_\ell^p e_{j_0}\|^2_{\varepsilon_0} - 9k^2\|\partial_\ell^p e_{j_0}\|_{L^2([0,2\pi])}.$$

When $p=0$ this is bounded by $\lambda_{j_0}(\ell)$ since e_{j_0} is unitary. When $p=1$ we need to express $\partial_\ell e_{j_0}$. By definition we have $(M_0(3k,\ell) - \lambda_{j_0}(\ell))e_{j_0}(3k,\ell)(y) = 0$. Differentiating this equation w.r.t. ℓ we get

$$(-\partial_\ell \lambda_{j_0}(\ell) + \partial_\ell M_0(3k,\ell))e_{j_0} + (M_0(3k,\ell) - \lambda_{j_0}(\ell))\partial_\ell e_{j_0} = 0. \tag{C.1}$$

Multiplying scalarly by e_{j_0} gives the following bound for $\partial_\ell \lambda_{j_0}$:

$$\partial_\ell \lambda_{j_0} = (\partial_\ell M_0(3k,\ell)e_{j_0}, e_{j_0})_{\varepsilon_0} = -2i\left(\frac{\varepsilon_0}{\varepsilon}(\partial_y + i\ell)e_{j_0}, e_{j_0}\right) \le 2\sup_x \frac{\varepsilon_0}{\varepsilon}\|(\partial_y + i\ell)e_{j_0}\|_{L^2([0,2\pi])}.$$

Since the first term in (C.1) is orthogonal to e_{j_0} we get $\partial_\ell e_{j_0}$ by inverting $(M_0(3k,\ell) - \lambda_{j_0}(\ell))|_{e_{j_0}^\perp}$ whose operator norm in $L^2([0,2\pi])$ is bounded.

2. Estimating $(D_\ell^{a'}(y)e_{j_0}, D_\ell^{b'}(y)\widetilde{P}_{0,3}(\ell))_{\varepsilon_0}$. First, note that

$$\partial_\ell^{b'}\widetilde{P}_{0,3} = (-i)^{b'}\widetilde{y^{b'}P_{0,3}}.$$

Then, using the Parseval identity in Definition 2.4 we get, when $b'=1$

$$\int_{-1/2}^{1/2}(e_{j_0}, \partial_\ell \widetilde{P}_{0,3})^2_{\varepsilon_0} d\ell \le \|\widetilde{yP_{0,3}}\|^2_{L^2_{\varepsilon_0}(\Gamma)} = \|yP_{0,3}\|^2_{L^2(\mathbb{R})} < \infty,$$

where $\Gamma = [-1/2,1/2]\times[0,2\pi]$. Thus $(e_{j_0}, \partial_\ell \widetilde{P}_{0,3})_{\varepsilon_0}$ is bounded almost everywhere and there is some point, say $\ell = 0$ at which $(e_{j_0}, \partial_\ell \widetilde{P}_{0,3})^2_{\varepsilon_0} < \|yP_{0,3}\|^2_{L^2(\mathbb{R})}$. Thus, the sup norm of $(e_{j_0}(\ell), \partial_\ell \widetilde{P}_{0,3}(\ell))^2_{\varepsilon_0}$ is bounded by $\|yP_{0,3}\|^2_{L^2(\mathbb{R})}$ plus

$$\int_0^\ell \partial_\ell (e_{j_0}, \partial_\ell \widetilde{P}_{0,3})^2_{\varepsilon_0} d\ell \le 2\|yP_{0,3}\|_{L^2(\mathbb{R})}\left(\|y^2P_{0,3}\|_{L^2(\mathbb{R})} + \|(\partial_\ell e_{j_0}, \partial_\ell \widetilde{P}_{0,3})_{\varepsilon_0}\|_{L^2(-1/2,1/2)}\right).$$

The last term is bounded by $\|\partial_\ell e_{j_0}\|_{\varepsilon_0}\|yP_{0,3}\|_{L^2(\mathbb{R})}$ by the Cauchy-Schwarz inequality and $\|\partial_\ell e_{j_0}\|_{\varepsilon_0}$ was estimated in the previous item.

If $a'=1$ the same analysis applies (one has to express the second derivative of e_{j_0} w.r.t. ℓ). Finally, note that we replaced the derivative $D_\ell(y)$ by ∂_ℓ. The missing y makes no problem since it is bounded.

3. Estimating $(D_\ell(y)p_{j_0}P_{0,3}, P_{0,3})_\varepsilon$.

Those projectors are defined in three parts: $|y|>a$ and $|y|<a$ which is the support of $\tilde{\varepsilon}$ (see Appendix B). For $\pm y > a$ one has

$$p_{j_0}(3k,\ell)P_{0,3} = c_\mp(\lambda_{j_0}(\ell))e_{j_0}(\ell,y)\partial_\ell \lambda_{j_0}(\ell).$$

The derivative of this expression requires to compute the derivative $\partial_\lambda c_\mp(\lambda)$ which requires in turn to compute $Q'(\lambda)$ and $(P(\lambda)^{-1})'$ where $Q(\lambda)$ is the fundamental matrix of the first order equation obtained from the operator $(M(3k)-\lambda)$ and $P(\lambda)$ is a matrix related to the values of p_{j_0} at $\pm a$. But those matrices are holomorphic in λ outside the zeroes of $P(\lambda)$ which is the case from Assumption 2.9. Since $P_{0,3}$ shows up through an integration over $y\in[-a,a]$ we see that $(\partial_\lambda^a p_{j_0}P_{0,3}, P_{0,3})_\varepsilon$ is bounded by $c_{j_0}\|P_{0,3}\|_\varepsilon$ where c_{j_0} is a constant depending only on the band j_0. Similar bounds exist when we replace the derivative ∂_ℓ by the multiplicator y. Finally, for $|y|<a$ we have a similar expression but the dependence in y is now given through $Q(\lambda,y)$. The derivatives $\partial_\lambda^a Q(\lambda,y)$ are bounded uniformly in y since they belong to $[-a,a]$.

□

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